

=> fil hcaplus  
 FILE 'HCAPLUS' ENTERED AT 09:59:03 ON 06 MAR 2006  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

8/17/01

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 6 Mar 2006 VOL 144 ISS 11  
 FILE LAST UPDATED: 5 Mar 2006 (20060305/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
 =>

=> d stat que  
 L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?  
 L2 SEL PLU=ON L1 1- CHEM : 100 TERMS  
 L3 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L2  
 L4 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L3 OR NOOTKATON?  
 L5 7087 SEA FILE=HCAPLUS ABB=ON PLU=ON (TICKS/CV OR ACARI/CV) OR  
 TICK OR ACARI OR ANTITICK? OR ANTIACARI?  
 L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND L5

=>  
 =>

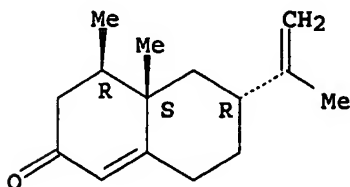
=> d ibib abs hitstr 16 1-6 .

L6 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:904357 HCAPLUS  
 DOCUMENT NUMBER: ~~143-224148~~  
 TITLE: Arthropod control compositions comprising eremophilane sesquiterpene and dialkylphenol  
 INVENTOR(S): Dolan, Marc C.; Panella, Nicholas A.; Dietrich, E. B. Gabrielle; Karchesy, Joseph J.; Maupin, Gary O.  
 PATENT ASSIGNEE(S): The Govt. of the U.S.A, Dept of Health and Human Services, Centers of Disease Control and Prevention, USA; State of Oregon Acting by and Through the State Board of High Education Oregon State University  
 SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 450,024.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

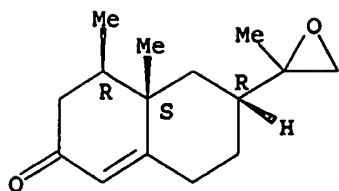
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005187289	A1	20050825	US 2005-115849	20050426
WO 2002050053	A2	20020627	WO 2001-US47736	20011207
WO 2002050053	A3	20030116		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004077713	A1	20040422	US 2003-450024	20031110
PRIORITY APPLN. INFO.:			US 2000-254311P	P 20001208
			WO 2001-US47736	W 20011207
			US 2003-450024	A2 20031110
AB	Compns. for controlling an arthropod pest population that include an eremophilane sesquiterpene pest control agent (such as, nootkatone or 13-hydroxy-valencene) and a dialkylphenol pesticide (such as carvacrol) are disclosed. The compds. present in the compns. may be isolated from natural sources, semi-synthesized from naturally occurring compds., or completely synthesized. The pest control compns. may be applied directly to a pest or the locus of a pest, and function as topical or ingestible pest toxins.			
IT	4674-50-4P, Nootkatone RL: AGR (Agricultural use); BUU (Biological use, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and extraction from Alaska yellow cedar and grapefruit oil as insecticide and acaricide)			
RN	4674-50-4 HCAPLUS			
CN	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)			

Absolute stereochemistry.



IT	438536-22-2P RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation as insecticide and acaricide)			
RN	438536-22-2 HCAPLUS			
CN	2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(2-methyloxiranyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)			

Absolute stereochemistry.



L6 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:514138 HCAPLUS  
 TITLE: Potential of Natural Forest Products for the Prevention of Lyme Disease  
 AUTHOR(S): Piesman, Joseph; Dolan, Marc C.  
 CORPORATE SOURCE: Division of Vector-Borne Infectious Diseases, Centers for Disease Control and Prevention, Fort Collins, CO, 80522, USA  
 SOURCE: Abstracts, 60th Northwest Regional Meeting of the American Chemical Society, Fairbanks, AK, United States, June 15-18 (2005); GEN-018. American Chemical Society: Washington, D. C.  
 CODEN: 69GZQM  
 DOCUMENT TYPE: Conference; Meeting Abstract  
 LANGUAGE: English

AB The incidence of Lyme disease continues to increase in the U.S. In 1991, when Lyme disease first became a nationally reportable disease to the Centers for Disease Control and Prevention (CDC), a total of 9,470 cases were reported; in contrast, by 2002 a total of 23,763 cases were reported, >2.5X the total in 1991. Traditional area-wide acaricides can be highly effective in killing nymphal Ixodes scapularis, with >95% of nymphs killed in studies using cyfluthrin, deltamethrin, or carbaryl. The majority of residents living in households within the area hyperendemic for Lyme disease will not, however, consider the use of area-wide acaricides. A survey of communities in 4 states (Connecticut, Massachusetts, New Jersey & New York) demonstrated that <25% of the populace have used area-wide acaricides on their own property. In searching for alternative methods of reducing Lyme disease risk, laboratory bioassays were conducted to determine the

activity of 15 natural products isolated from the essential oil components extracted from the heartwood of Alaska yellow cedar (AYC) (Chamaecyparis nootkatensis) against I. scapularis nymphs. Nootkatone from AYC was the most effective biocide of the eremophilane sesquiterpenes with an LC50 value of 0.029 mg/mL. Residual LC50 values for Nootkatone did not differ significantly at 4 wk post-treatment from the observations made at the initial 24 h treatment. Nymphal tick repellent bioassays resulted in 5 natural product compds. with repellent dose (RD50) values lower than Deet. The most active compound, valencene-13-ol, had an RD50 of 0.03 mg/mL at 4 h compared to 3.8 mg/mL for Deet. The ability of these natural products to kill and repel ticks at relatively low concns. may represent a future alternative to the use of synthetic pesticides.

L6 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:484325 HCAPLUS  
 DOCUMENT NUMBER: 144:1573  
 TITLE: Use of novel compounds for pest control: insecticidal and acaricidal activity of essential oil components from heartwood of Alaska yellow cedar  
 AUTHOR(S): Panella, Nicholas A.; Dolan, Marc C.; Karchesy, Joseph

CORPORATE SOURCE: J.; Xiong, Yeping; Peralta-Cruz, Javier; Khasawneh, Mohammad; Montenieri, John A.; Maupin, Gary O. Division of Vector-Borne Infectious Diseases, National Center for Infectious Diseases, Centers for Disease Control and Prevention, Public Health Service, U.S. Department of Health and Human Services, Fort Collins, CO, 80522, USA

SOURCE: Journal of Medical Entomology (2005), 42(3), 352-358  
CODEN: JMENA6; ISSN: 0022-2585

PUBLISHER: Entomological Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

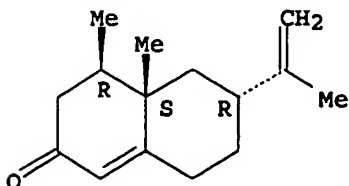
AB Laboratory bioassays were conducted to determine the activity of 15 natural products isolated from essential oil components extracted from the heartwood of Alaska yellow cedar, *Chamaecyparis nootkatensis* (D. Don) Spach., against *Ixodes scapularis* Say nymphs, *Xenopsylla cheopis* (Rothchild), and *Aedes aegypti* (L.) adults. Four of the compds. from the essential oil were identified as monoterpenes, 5 as eremophilane sesquiterpenes, 5 as eremophilane sesquiterpene derivs. from valencene and nootkatone, and one as a sesquiterpene outside the eremophilane parent group. Carvacrol was the only monoterpene that demonstrated biocidal activity against ticks, fleas, and mosquitoes with LC50 values after 24 h of 0.0068, 0.0059, and 0.0051% (wt:vol), resp. Nootkatone from Alaska yellow cedar was the most effective of the eremophilane sesquiterpenes against ticks (LC50 = 0.0029%), whereas the nootkatone grapefruit extract exhibited the greatest biocidal activity against fleas (LC50 = 0.0029%). Mosquitoes were most susceptible to one of the derivs. of valencene, valencene-13-aldehyde (LC50 = 0.0024%), after 24 h. Bioassays to determine residual activity of the most effective products were conducted at 1, 2, 4, and 6 wk after initial treatment. Residual LC50 values for nootkatone did not differ significantly at 4 wk posttreatment from the observations made at the initial 24-h treatment. The ability of these natural products to kill arthropods at relatively low concns. represents an alternative to the use of synthetic pesticides for control of disease vectors.

IT 4674-50-4P, Nootkatone 438536-22-2P, Nootkatone 11,12 epoxide  
RL: AGR (Agricultural use); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation); USES (Uses) (insecticidal and acaricidal activity of essential oil components from heartwood of Alaska yellow cedar)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

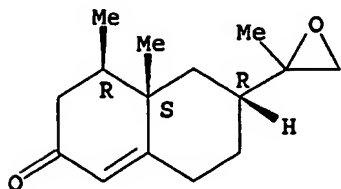
Absolute stereochemistry.



RN 438536-22-2 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(2-methyloxiranyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:18729 HCAPLUS  
 DOCUMENT NUMBER: 140:37445  
 TITLE: Dihydronootkatone and tetrahydronootkatone as arthropod repellents  
 INVENTOR(S): Zhu, Betty C. R.; Henderson, Gregg; Laine, Roger A.  
 PATENT ASSIGNEE(S): Board of Supervisors of Louisiana State University and Agricultural and Mechanical College, USA  
 SOURCE: U.S. Pat. Appl. Publ., 10 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004005343	A1	20040108	US 2002-189631	20020703
US 6897244	B2	20050524		
WO 2004031140	A2	20040415	WO 2003-US20747	20030701
WO 2004031140	A3	20040708		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2005171213 A1 20050804 US 2005-53472 20050208

PRIORITY APPLN. INFO.: US 2002-189631 A 20020703

AB Two derivs. of nootkatone, tetrahydronootkatone and 1,10-dihydronootkatone, are surprisingly effective as repellents of termites and mosquitoes. Tetrahydronootkatone and 1,10-dihydronootkatone were shown to effectively repel termites at concns. as low as 2 µg/mL and 12.5 µg/mL, resp. Tetrahydronootkatone was shown to repel mosquitos at a concentration of 5%. Tetrahydronootkatone is an effective repellent of termites either by itself or as an addition to other substrates, including mulches made from wood products or other cellulose-containing material. Tetrahydronootkatone or 1,10-dihydronootkatone can be used to protect construction wood from

attack by Formosan subterranean termites, either alone or used in combination with other compds. known to repel termites. It is also believed that these compds. will prove effective in repelling ants, ticks, and cockroaches. These derivs. of nootkatone are non-toxic to humans and other mammals and environmentally safe.

IT 20489-53-6, 1,10-Dihydronootkatone

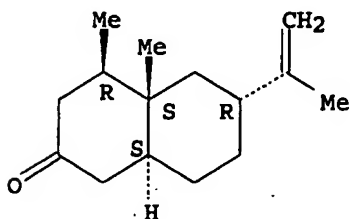
20489-54-7, Tetrahydronootkatone

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(arthropod repellent)

RN 20489-53-6 HCAPLUS

CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R,8aS) - (9CI) (CA INDEX NAME)

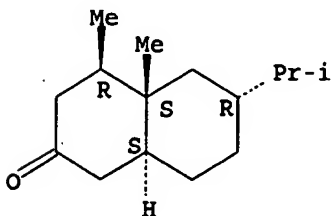
Absolute stereochemistry.



RN 20489-54-7 HCAPLUS

CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethyl)-, (4R,4aS,6R,8aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



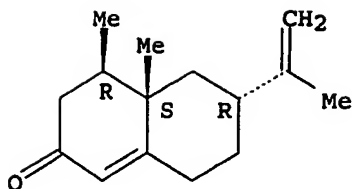
IT 4674-50-4, Nootkatone

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(in arthropod repellent compns. comprising dihydronootkatone and/or tetrahydronootkatone)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:300627 HCAPLUS

DOCUMENT NUMBER: 138:299241

TITLE: Extracts of vetiver oil as repellent and toxicant to ants, ticks, and cockroaches

INVENTOR(S): Henderson, Gregg; Heumann, Donald O.; Laine, Roger A.; Maistrello, Lara; Zhu, Betty C. R.; Chen, Feng

PATENT ASSIGNEE(S): Board of Supervisors of Louisiana State University and Agricultural and Mechanical College, USA

SOURCE: U.S. Pat. Appl. Publ., 13 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003073748	A1	20030417	US 2001-932555	20010817
US 6906108	B2	20050614		
US 2004157935	A1	20040812	US 2004-769830	20040202
			US 2001-932555	A3 20010817

PRIORITY APPLN. INFO.:

AB Exts. of vetiver oil were found to be significant repellents and toxicants of ants, ticks, and cockroaches. Nootkatone was shown to significantly decrease ant invasion and increase mortality in fire ants. Nootkatone is an effective repellent and toxicant of ants either by itself or as an addition to other substrates, including mulches made from vetiver grass roots, diatomaceous earth, alumina, silica, clays; building materials made from either aluminum or wood; and other suitable solid substances. Nootkatone was also a repellent and toxicant to ticks; and a repellent to cockroaches. Nootkatone is non-toxic to humans and other mammals and is environmentally safe. In addition, other components of vetiver oil, specifically  $\alpha$ -cedrene, zizanol and bicyclovetivenol, are effective against ants, ticks, and cockroaches.

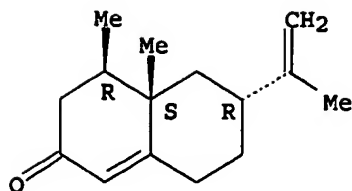
IT 4674-50-4, Nootkatone

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(repellent and toxicant to ants, ticks, and cockroaches)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

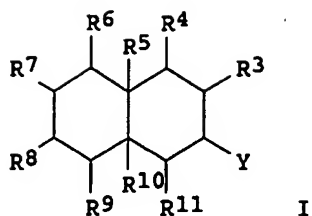
Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:487546 HCAPLUS  
 DOCUMENT NUMBER: 137:59007  
 TITLE: Eremophilane sesquiterpenes pesticides for arthropod control  
 INVENTOR(S): Maupin, Gary O.; Karchesy, Joseph; Panella, Nicholas A.; Dolan, Marc C.  
 PATENT ASSIGNEE(S): The Government of the United States of America, Department of Health and Human Services, USA  
 SOURCE: PCT Int. Appl., 89 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050053	A2	20020627	WO 2001-US47736	20011207
WO 2002050053	A3	20030116		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2431548	AA	20020627	CA 2001-2431548	20011207
AU 2002045095	A5	20020701	AU 2002-45095	20011207
EP 1355895	A2	20031029	EP 2001-993241	20011207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004077713	A1	20040422	US 2003-450024	20031110
US 2005176818	A1	20050811	US 2005-105807	20050413
US 2005187289	A1	20050825	US 2005-115849	20050426
PRIORITY APPLN. INFO.:				
			US 2000-254311P	P 20001208
			WO 2001-US47736	W 20011207
			US 2003-450024	A1 20031110
OTHER SOURCE(S): MARPAT 137:59007				
GI				



AB The eremophilane sesquiterpenes I (C1R6C10R5 = Q; Y = C11R1R2R12 or Q1; R1-12 = H, O, OH, lower aliphatic alc. or thiol, etc.; R1-12 satisfy valence requirements) are pesticides for arthropod control. The compds. have minimal adverse or toxic effects on humans, animals, and the natural environment. The compds. may be isolated from natural sources, semi-synthesized from naturally occurring compds., or completely synthesized. The compds. may be applied directly to a pest, or the locus of a pest, and function as topical or ingestible toxins. 13-Hydroxy-valencene, valencene-11,12-epoxide, valencene-13-aldehyde, and nootkatone-1,10-11,12-diepoxy are exemplary compds.

IT 438536-22-2P

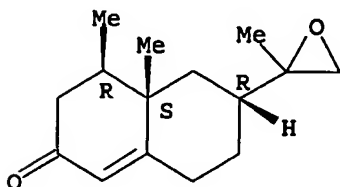
RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation as pesticide for arthropod control)

RN 438536-22-2 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(2-methyloxiranyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 4674-50-4, Nootkatone

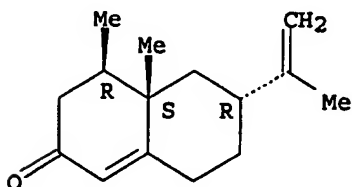
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant in preparation of nootkatone epoxide pesticides for arthropod control)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> => d stat que 18

L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?  
 L2 SEL PLU=ON L1 1- CHEM : 100 TERMS  
 L3 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L2  
 L4 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L3 OR NOOTKATON?  
 L5 7087 SEA FILE=HCAPLUS ABB=ON PLU=ON (TICKS/CV OR ACARI/CV) OR  
 TICK OR ACARI OR ANTITICK? OR ANTIACARI?  
 L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND L5  
 L7 194193 SEA FILE=HCAPLUS ABB=ON PLU=ON PESTICIDES/CV OR ACARICIDES/CV  
 OR INSECTICIDES/CV OR RODENTICIDES/CV REPELLENTS/CV OR  
 PESTICIDE OR INSECTICIDE OR RODENTICIDE OR REPELLENT  
 L8 16 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND L7) NOT L6

=> d ibib abs hitstr 18 1-16

L8 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:1102086 HCAPLUS  
 DOCUMENT NUMBER: 143:192667  
 TITLE: Biological lemon and sweet orange essential oil  
 composition  
 AUTHOR(S): Verzera, A.; Trozzi, A.; Dugo, G.; Di Bella, G.;  
 Cotroneo, A.  
 CORPORATE SOURCE: Dipartimento di Chimica Organica e Biologica, Facolta  
 di Scienze, Universita di Messina, Italy  
 SOURCE: Flavour and Fragrance Journal (2004), 19(6), 544-548  
 CODEN: FFJOED; ISSN: 0882-5734  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The volatile fraction composition of sweet orange and lemon oils obtained using  
 biol. and traditional cultivation is reported. The oils came from Sicily  
 and were industrially obtained. The aim of the research was to establish  
 whether the use of pesticides in citrus cultivation could  
 influence the essential oil composition. The volatile fraction was analyzed by  
 HRGC and HRGC-MS. The content of organophosphorus and organochlorine  
 pesticides was determined by HRGC-FPD and HRGC-ECD. Differences in the  
 oil composition resulted, especially in the content of carbonyl compds.; the  
 results

obtained, altogether, show that the biol. oils are of higher quality in  
 terms of their composition than traditional ones.

IT 4674-50-4, Nootkatone

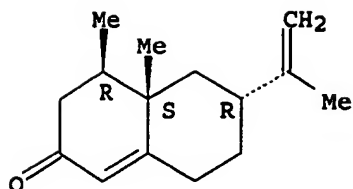
RL: BSU (Biological study, unclassified); FFD (Food or feed use); BIOL  
 (Biological study); USES (Uses)

(lemon and sweet orange essential oil composition from cultivation with and  
 without pesticides)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:186392 HCAPLUS

DOCUMENT NUMBER: 140:419294

TITLE: Toxicity and behavioral effects of nootkatone, 1,10-dihydronootkatone, and tetrahydronootkatone to the formosan subterranean termite (Isoptera: Rhinotermitidae)

AUTHOR(S): Ibrahim, Sanaa A.; Henderson, Gregg; Zhu, Betty C. R.; Fei, Huixin; Laine, Roger A.

CORPORATE SOURCE: Department of Plant Protection, Faculty of Agriculture, Minia University, Minia, Egypt

SOURCE: Journal of Economic Entomology (2004), 97(1), 102-111  
CODEN: JEENAI; ISSN: 0022-0493

PUBLISHER: Entomological Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

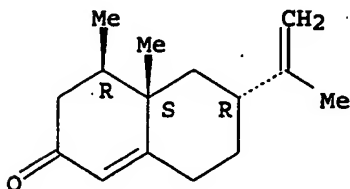
AB Toxicity and behavioral effects of nootkatone and two of its derivs., 1,10-dihydronootkatone and tetrahydronootkatone, to *Coptotermes formosanus* Shiraki were investigated on workers from two different colonies by using topical application assays, repellency assays, and sand barrier assays. The acute toxicity of the nootkatones on workers from both colonies increased as the saturation of the mol. increased, but the difference was significant for only one colony. The results of the repellency assays showed a similar trend of efficiency; the threshold concentration for significant repellency was four-fold higher in nootkatone treatments (50 ppm) than in the reduced derivs. 1,10-dihydronootkatone or tetrahydronootkatone (12.5 ppm). In sand barrier assays, a concentration of 100 ppm of any of the three chems. significantly reduced termite survival, tunnel building, and food consumption after a 12-d exposure. Termites preexposed to 100 ppm nootkatone-treated sand and placed in containers without nootkatone for 15 d continued to exhibit abnormal feeding and digging behaviors; survivorship, tunneling, and feeding activities were significantly reduced by 83.5, 63.2, and 95.4% resp. Termites pretreated for 12 d at concns. of 50 and 75 ppm nootkatone and tetrahydronootkatone returned to normal digging activity after they were removed from the treatments, but their feeding activity was significantly reduced.

IT 4674-50-4, Nootkatone 20489-53-6, 1, 10-Dihydronootkatone 20489-54-7, Tetrahydronootkatone  
RL: BSU (Biological study, unclassified); BIOL (Biological study) (toxicity and behavioral effects of nootkatone, 1, 10-dihydronootkatone, and tetrahydronootkatone to formosan subterranean termite)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

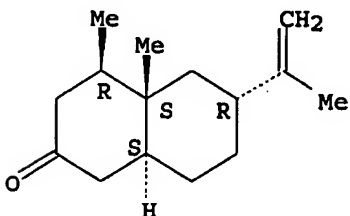
Absolute stereochemistry.



RN 20489-53-6 HCAPLUS

CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R,8aS)- (9CI) (CA INDEX NAME)

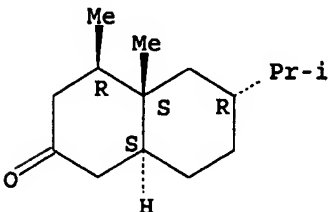
Absolute stereochemistry.



RN 20489-54-7 HCAPLUS

CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethyl)-, (4R,4aS,6R,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

46

THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:980198 HCAPLUS

DOCUMENT NUMBER: 140:266111

TITLE: Structure-activity of valencenoid derivatives and their repellence to the Formosan subterranean termite  
AUTHOR(S): Zhu, Betty C. R.; Henderson, Gregg; Sauer, Anne M.; Yu, Ying; Crowe, William; Laine, Roger A.

CORPORATE SOURCE: Louisiana State University Agricultural Center, Louisiana Agricultural Experiment Station, Department of Entomology, Louisiana State University, Baton

SOURCE: Rouge, LA, 70808, USA  
Journal of Chemical Ecology (2003), 29(12); 2695-2701  
CODEN: JCECD8; ISSN: 0098-0331  
PUBLISHER: Kluwer Academic/Plenum Publishers  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 140:266111

AB Eight valencenoid derivs. were prepared and evaluated for their repelling activity against Formosan subterranean termites, *Coptotermes formosanus* Shiraki. Among them, 1,10-dihydronootkatone was the strongest repellent, and valencene was the weakest. Results of the structure-repellency relationships indicated: (1) reduction of the ketone group to the alc. on position 2 of **nootkatone** curtailed the activity; (2) because of the low activity of valencene relative to **nootkatone**, the ketone group was essential for repellent activity; (3) reduction of the 1,10 double bond (1,10-dihydronootkatone and tetrahydronootkatone) produced compds. more repellent than **nootkatone**; (4) the isopropenyl group probably does not participate in binding as evidenced by no significant difference in the repellent activity among **nootkatone** (double bond between position 11 and 12), **isonootkatone** (double bond between position 7 and 11), and **11,12-dihydronootkatone**.

IT 4674-50-4, **Nootkatone** 20489-53-6, 1, 10-Dihydronootkatone 20489-54-7, Tetrahydronootkatone)

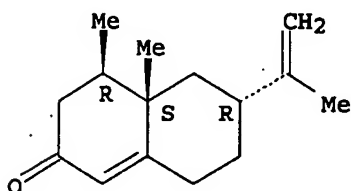
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(Formosan subterranean termite repellent)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

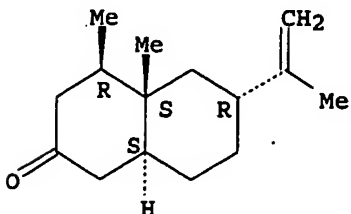
Absolute stereochemistry.



RN 20489-53-6 HCAPLUS

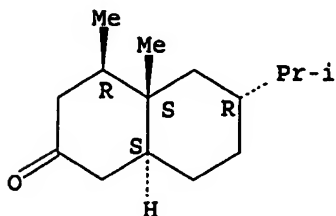
CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



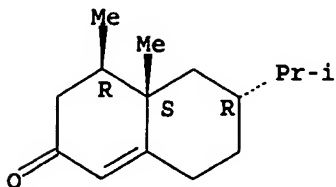
RN 20489-54-7 HCAPLUS  
 CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethyl)-,  
 (4R,4aS,6R,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



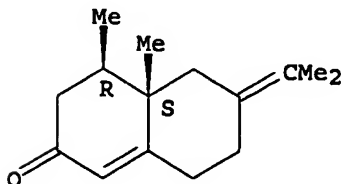
IT 5195-69-7P, 11,12-Dihydronootkatone  
 15764-04-2P, Isonootkatone)  
 RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation); USES (Uses)  
 (preparation as Formosan subterranean termite repellent)  
 RN 5195-69-7 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:358482 HCAPLUS  
 DOCUMENT NUMBER: 139:188609  
 TITLE: The sesquiterpenoid nootkatone and the  
 absolute configuration of a dibromo derivative  
 AUTHOR(S): Sauer, Anne M.; Fronczek, Frank R.; Zhu, Betty C. R.;

CORPORATE SOURCE: Crowe, William E.; Henderson, Gregg; Laine, Roger A.  
Department of Chemistry, Louisiana State University,  
Baton Rouge, LA, 70803-1804, USA

SOURCE: Acta Crystallographica, Section C: Crystal Structure  
Communications (2003), C59(5), o254-o256  
CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Blackwell Munksgaard

DOCUMENT TYPE: Journal

LANGUAGE: English

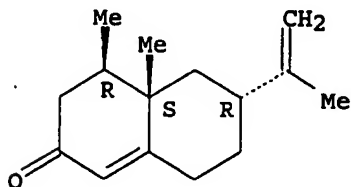
AB Nootkatone, or (4R,4aS,6R)-4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)naphthalen-2(3H)-one, C<sub>15</sub>H<sub>22</sub>O, a sesquiterpene with strong repellent properties against Formosan subterranean termites and other insects, has the valencene skeleton. The dibromo derivative (1S,3R,4S,4aS,6R,8aR)-1,3-dibromo-6-isopropyl-4,4a-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-2-one, C<sub>15</sub>H<sub>24</sub>Br<sub>2</sub>O, has two independent mols. in the asym. unit, which differ in the rotation of the iso-Pr group with respect to the main skeleton. Crystallog. data are given. The C-Br distances are in the range 1.950(4)-1.960(4) Å. Both independent mols. form zigzag chains, with very short intermol. carbonyl-carbonyl interactions, having the perpendicular motif and O...C distances of 2.886(6) and 2.898(6) Å. These chains are flanked by intermol. Br...Br interactions of distances in the range 4.067(1)-4.218(1) Å. The absolute configuration of the dibromo derivative was determined, from which that of nootkatone was inferred.

IT 4674-50-4, Nootkatone  
RL: PRP (Properties)  
(crystal structure of)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:97811 HCAPLUS

DOCUMENT NUMBER: 138:118831

TITLE: Environmentally safe insect repellent  
composition containing D-limonene and essential oils

INVENTOR(S): Fried, Howard L.; Khazan, Donna; Morales, Mark N.

PATENT ASSIGNEE(S): The 54 Group, Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 6 pp., Cont.-in-part of U. S. Ser. No. 874,361.  
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003026823	A1	20030206	US 2002-162009	20020604
US 2002034556	A1	20020321	US 2001-874361	20010605
EP 1404352	A1	20040407	EP 2002-753333	20020605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2005249768	A1	20051110	US 2005-87389	20050322
PRIORITY APPLN. INFO.:				
			US 2000-209346P	P 20000605
			US 2001-874361	A2 20010605
			US 2002-162009	A 20020604
			WO 2002-US17583	W 20020605

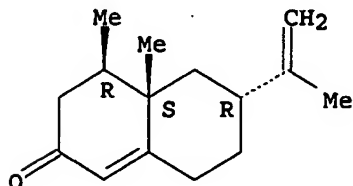
AB An insect repellent composition contains citronella oil, D-limonene, 2 or more synergists, and 3 or more essential oils as the active ingredients. The preferred essential oils are geranium oil, rosemary oil and peppermint oil, but other essential oils may be used. In the preferred embodiment the synergists are aldehyde C-14 and aldehyde C-18. As desired, vanillin may be used as a stabilizer, and fragrances, fragrance enhancers and surfactants may be utilized.

IT 4674-50-4, Nootkatone  
 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); MOA (Modifier or additive use); BIOL (Biological study); USES (Uses)  
 (synergist in environmentally safe insect repellent composition containing D-limonene and essential oils)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:43495 HCAPLUS

DOCUMENT NUMBER: 138:233376

TITLE: Comparative effects of vetiver oil, nootkatone and disodium octaborate tetrahydrate on Coptotermes formosanus and its symbiotic fauna

AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.

CORPORATE SOURCE: Department of Entomology, Louisiana State University Agricultural Center, Baton Rouge, LA, 70803, USA

SOURCE: Pest Management Science (2003), 59(1), 58-68  
 CODEN: PMSCFC; ISSN: 1526-498X

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The potential of vetiver oil and nootkatone as wood treatments against Coptotermes formosanus Shiraki was examined by assessing the effects on termite tunneling, feeding activity and survival, and the consequences on the symbiont protozoa responsible for wood digestion. Comparisons were

made with non-treated wood (control), wood treated with the borate compound Tim-Bor (a commonly used lumber preservative) and absence of a food source (starved termites), using choice and no-choice tests. All wood slices were prepared at the same time using a 10 g liter-1 solution of each substance and were tested in four different sessions over one year to investigate longevity of the effects. Termites had to tunnel through sand to exploit the food sources, consisting of two wood slices, placed on opposite sides of the exptl. enclosure. No-choice tests showed that in the presence of vetiver oil or **nootkatone**, tunneling activity was always the lowest; wood consumption, termite survival and flagellate nos. and species distribution were significantly different from the control and similar to the results obtained for starved termites and with Tim-Bor-treated wood. **Nootkatone** neg. affected termites for 12 mo and was longer lasting than vetiver oil. In choice tests, when vetiver oil or **nootkatone** were present, termites exhibited a significant preference for non-treated wood. Our results confirmed both the toxicity and absence of repellency of Tim-Bor. Vetiver oil and especially **nootkatone** affected Formosan subterranean termites and their protozoa, acting as arrestants, repellents and feeding deterrents, and represent a promising natural alternative for the control of this invasive pest..

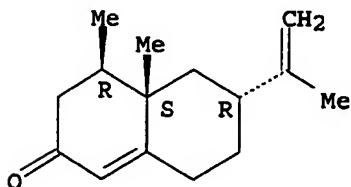
IT 4674-50-4, **Nootkatone**

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
(effects on *Coptotermes formosanus* and its symbiotic fauna)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:679014 HCAPLUS

DOCUMENT NUMBER: 138:316185

TITLE: Comparative chemical and biological investigations of certain essential oils belonging to families Asteraceae, Lamiaceae and Graminae

AUTHOR(S): Hifnawy, Mohamed S.; Rashwan, Omar A.; Rabeh, Mohamed A.

CORPORATE SOURCE: Department of Pharmacognosy, Faculty of Pharmacy, Cairo, 11562, Egypt

SOURCE: Bulletin of the Faculty of Pharmacy (Cairo University) (2001), 39(2), 35-53

CODEN: BFPHA8; ISSN: 1110-0931

PUBLISHER: Cairo University, Faculty of Pharmacy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The demand for pesticidal and antimicrobial compds. of natural origin are now of great importance as they are more safe, more selective and

biodegradable. Identification of different constituents of *Artemisia monosperma* Del., *A. judaica* L., *A. herba alba* Asso., *Achillea fragrantissima* (Forsk) Sch.Bip., *Tanacetum santolinoides* (D.C.) Feinbr and Fertig, *Cymbopogon citratus* Stapf. and *C. nardus* Rendle, *Ocimum basilicum* L. and *O. canum* Sims. were performed using GC and GC/MS anal. The antibacterial activity against *Bacillus subtilis* and *Escherichia coli*, larvicidal activity against *Culex pipiens* mosquito and cotton leafworm *Spodoptera littoralis* (Biosd.) larvae, insecticidal activity against houseflies *Musca domestica* L. and rodenticidal activity against white mice *Mus musculus* were performed. The oil of *T. santolinoides* showed the highest antibacterial activity against both bacterial species tested followed by *C. nardus*, *C. citratus*, *A. fragrantissima* and *A. judaica* oils, while that of *O. basilicum* showed no antibacterial activity. Others oils had nonsignificant antibacterial activity against both bacterial species tested. The oil of *T. santolinoides* was the most potent against all biol. species tested, followed by *A. monosperma* against *Culex pipiens* mosquito larvae, *O. basilicum* against cotton leafworm *Spodoptera littoralis* (Biosd.) larvae and houseflies *Musca domestica* L. insects and *A. judaica* against white mice *Mus musculus*.

IT 15764-04-2,  $\alpha$  -Vetivone

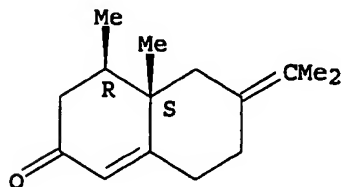
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(component of pesticidal essential oils from Asteraceae, Lamiaceae and Graminae)

RN 15764-04-2 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:613344 HCAPLUS

TITLE: Termiticidal activity of essential oils against the formosan subterranean termite

AUTHOR(S): Chen, Feng; Zhu, Betty R. C.; Henderson, Gregg; Fei, Huixin; Laine, Roger; Wang, Xi

CORPORATE SOURCE: Department of Food Science and Human Nutrition, Clemson University, Clemson, SC, 29634, USA

SOURCE: Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002), AGFD-107. American Chemical Society: Washington, D. C.

CODEN: 69CZPZ

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Termiticidal activity of six essential oils from vetiver grass, cassia leaf, clove bud, cedarwood, lemon grass, and geranium, were investigated against the Formosan subterranean termite *Coptotermes formosanus*. Vetiver

oil and Clove bud oil in the controlled conditions showed the most effective repellency and toxicity, resp. In this study, nootkatone from vetiver oil was also found to possess potent repellent and toxic activity against the termite.

L8 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:29183 HCAPLUS

DOCUMENT NUMBER: 136:162704

TITLE: Efficacy of vetiver oil and nootkatone as soil barriers against formosan subterranean termite (Isoptera: Rhinotermitidae)

AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.

CORPORATE SOURCE: Department of Entomology, Louisiana State University Agricultural Center, Baton Rouge, LA, 70803, USA

SOURCE: Journal of Economic Entomology (2001), 94(6), 1532-1537

CODEN: JEENAI; ISSN: 0022-0493

PUBLISHER: Entomological Society of America

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Vetiver oil and its components nootkatone and cedrene were assessed as sand treatments for their efficacy to disrupt food recruitment by *Coptotermes formosanus* Shiraki. Termites were required to tunnel through sand treated with vetiver oil, nootkatone, cedrene, or untreated sand to reach a food source. Results showed that sand treated with vetiver oil or nootkatone disrupted termite tunneling behavior. As a consequence, after 21 d, wood consumption and termite survival were significantly lower compared with cedrene-treated or untreated sand treatments. Sand treated with vetiver oil or nootkatone at 100 µg/g substrate were effective barriers to termites.

IT 4674-50-4, Nootkatone

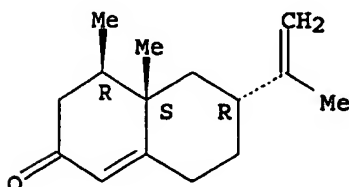
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(efficacy as soil barrier against formosan subterranean termite)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:473165 HCAPLUS

DOCUMENT NUMBER: 135:103770

TITLE: Nootkatone is a repellent for formosan subterranean termite (*Coptotermes formosanus*)

AUTHOR(S): Zhu, Betty C. R.; Henderson, Gregg; Chen, Feng; Maistrello, Lara; Laine, Roger A.

CORPORATE SOURCE: Department of Biological Sciences, Louisiana State University Agricultural Center, Louisiana Agricultural Experiment Station, Louisiana State University, Baton Rouge, LA, 70803, USA

SOURCE: Journal of Chemical Ecology (2001), 27(3), 523-531  
CODEN: JCECD8; ISSN: 0098-0331

PUBLISHER: Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

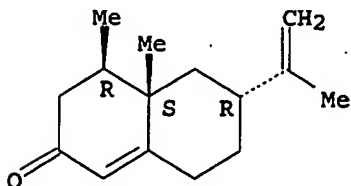
AB Nootkatone, a sesquiterpene ketone, isolated from vetiver oil is a strong repellent and toxicant to Formosan subterranean termites. The lowest effective concentration tested was 10 µg/g substrate. This is the first report of nootkatone being a repellent to insects.

IT 4674-50-4, Nootkatone  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(nootkatone as repellent for formosan subterranean termite)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:300439 HCAPLUS

DOCUMENT NUMBER: 134:306624

TITLE: Vetiver oil components as termite repellents and termiticides

INVENTOR(S): Henderson, Gregg; Laine, Roger A.; Heumann, Donald O.; Chen, Feng; Zhu, Betty C. R.

PATENT ASSIGNEE(S): Louisiana State University and Agricultural and Mechanical College, USA

SOURCE: PCT Int. Appl., 30 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028343	A1	20010426	WO 2000-US29006	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,				

Pryor 10\_769830 Claim 76

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
CA 2423950 AA 20010426 CA 2000-2423950 20001018  
EP 1221854 A1 20020717 EP 2000-972286 20001018  
EP 1221854 B1 20040303  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL  
AU 771326 B2 20040318 AU 2001-10969 20001018  
ES 2213052 T3 20040816 ES 2000-972286 20001018  
US 6890960 B1 20050510 US 2001-856760 20001018  
PRIORITY APPLN. INFO.: US 1999-160251P P 19991019  
WO 2000-US29006 W 20001018

AB Exts. of vetiver oil were found to significantly repel termites.  
Nootkatone was isolated and found to be a significant  
repellent and toxicant of termites. Nootkatone  
significantly decreased food consumption, decreased tunneling behavior,  
and increased mortality in termites. Nootkatone is an effective  
repellent and toxicant of termites either by itself or as an addition  
to other materials or substrates, including mulches made from vetiver  
grass roots or other wood products. Nootkatone can also be used  
to protect construction wood from attack by Formosan subterranean  
termites. Nootkatone as a repellent is nontoxic to  
humans and other mammals and is environmentally safe. In addition,  
 $\alpha$ -cedrene was found to be a weak termite repellent; and  
both zizanol and bicyclovetivenol were found to be repellents  
and toxicants of termites.

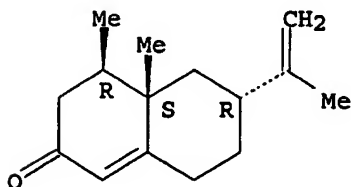
IT 4674-50-4, Nootkatone  
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
(Uses)

(vetiver oil components as termite repellents and  
termiticides)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:597259 HCAPLUS

DOCUMENT NUMBER: 133:173361

TITLE: Insecticidal Sesquiterpene from *Alpinia oxyphylla*  
against *Drosophila melanogaster*

AUTHOR(S): Miyazawa, Mitsuo; Nakamura, Yuji; Ishikawa, Yukio

CORPORATE SOURCE: Department of Applied Chemistry Faculty of Science and  
Engineering, Kinki University, Higashiosaka-shi Osaka,

SOURCE: 577-8502, Japan  
Journal of Agricultural and Food Chemistry (2000),  
48(8), 3639-3641  
CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

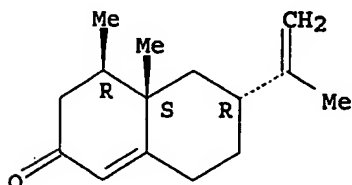
AB MeOH extract of *Alpinia oxyphylla* had insecticidal activity against larvae of *Drosophila melanogaster* Meigen. From the extract, an insecticidal compound was isolated by bioassay-guided fractionation and identified as nootkatone (I) by GC, GC-MS, and <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. In bioassays for insecticidal activity, I showed an LC<sub>50</sub> value of 11.5 μmol/mL of diet against larvae of *D. melanogaster* and an LD<sub>50</sub> value of 96 μg/adult against adults. Epinootkatol, however, showed slight insecticidal activity in both assays, indicating that the carbonyl group at the 2-position in I was the important function for enhanced activity of I.

IT 4674-50-4, Nootkatone  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(insecticidal sesquiterpene from *Alpinia oxyphylla* against *Drosophila melanogaster*)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:343658 HCAPLUS

DOCUMENT NUMBER: 130:348555

TITLE: Hematophagous insect repellents containing nootkatone and(or) valencene

INVENTOR(S): Takagi, Masahiro; Ogino, Kazumasa

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 14 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9925196	A1	19990527	WO 1998-JP5141	19981116
W: AU, CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

AU 9910536	A1	19990607	AU 1999-10536	19981116
JP 11240802	A2	19990907	JP 1998-325392	19981116
EP 1033076	A1	20000906	EP 1998-953056	19981116

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI

PRIORITY APPLN. INFO.:

JP 1997-314988	A	19971117
WO 1998-JP5141	W	19981116

AB Indoor hematophagous insect repellents with superior safety and valencene effectiveness comprise either an indoor fragrance containing at least 5%, or an aerosol containing at least 0.1%, of nootkatone, valencene or a mixture of these ingredients. Thus, 80 g water was mixed with carrageenan 2, locust bean gum 0.5 and propylene glycol 5 g and heated, and benzalkonium chloride 0.1, indigo carmine 0.05, and nootkatone 5 g were added, and the product was poured into a container. The solid room fragrance obtained by cooling was effective against *Culex pipiens pallens* females.

IT 4674-50-4, Nootkatone

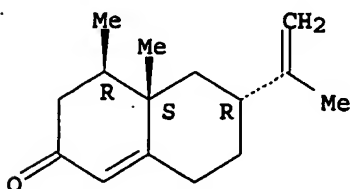
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(hematophagous insect repellents containing nootkatone and(or) valencene)

RN 4674-50-4 HCAPLUS

CN 2 (3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:208778 HCAPLUS

DOCUMENT NUMBER: 128:305149

TITLE: Repellents for control of Dermatophagoides

INVENTOR(S): Kusuki, Hirofumi; Fujii, Masashi

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10087409	A2	19980407	JP 1996-279823	19960913
PRIORITY APPLN. INFO.:			JP 1996-279823	19960913

AB The repellents contain ≥1 compound selected from 89 compound classes including essential oils, glycerides, plant exts., and esters (compds. of the 89 classes are described in the claim) and are applied at

0.01-100 weight% to household utensils, cosmetics, quasi-drugs, and topical preps. Tetrahydrolinalool showed repellent effects against Dermatophagoides pteronyssinus and D. farinae with a min. effective concentration of 1.0 weight%.

IT 4674-50-4, Nootkatone

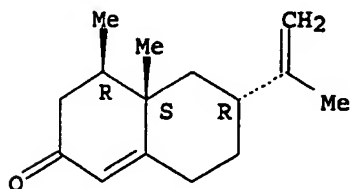
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); TEM (Technical or engineered material use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(repellents for control of Dermatophagoides)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:400558 HCAPLUS

DOCUMENT NUMBER: 125:51527

TITLE: Cockroach repellents containing sesquiterpenes

INVENTOR(S): Harima, Shoichi; Komai, Koichiro; Myake, Takayasu

PATENT ASSIGNEE(S): Tokiwa Kanpo Pharma, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08081306	A2	19960326	JP 1994-217066	19940912
PRIORITY APPLN. INFO.:			JP 1994-217066	19940912

AB Cockroach repellents contain (A) sesquiterpenes containing  $\geq 1$  groups chosen from CMe<sub>2</sub>OH, CHMeCH<sub>2</sub>OH, CH<sub>2</sub>OH, and cyclic ketones and  $\geq 1$  double bonds or (B) sesquiterpene alcs. containing 1 group chosen from CMe<sub>2</sub>OH and CHMeCH<sub>2</sub>OH and terminal methylene as active ingredients. Elemol at 1.0 g/m<sup>2</sup> showed 71-100% repellency against Blattella germanica and Periplaneta fuliginosa at 24 h after the application.

IT 4674-50-4P, Nootkatone

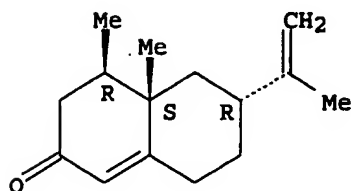
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cockroach repellents containing sesquiterpenes)

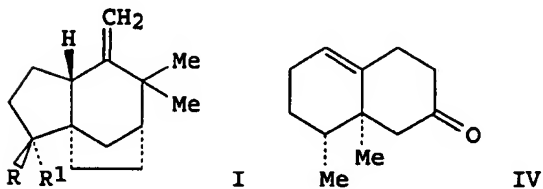
RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

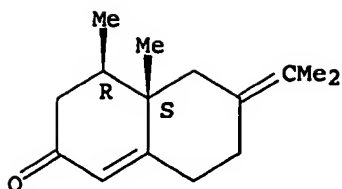


L8 ANSWER 16 OF 16 . HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1983:140523 HCAPLUS  
 DOCUMENT NUMBER: 98:140523  
 TITLE: Insect repellents from vetiver oil. Zizanal and epizizanal  
 AUTHOR(S): Jain, Subhash C.; Nowicki, Stephen; Eisner, Thomas; Meinwald, Jerrold  
 CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853, USA  
 SOURCE: Tetrahedron Letters (1982), 23(45), 4639-42  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Chromatog. of vetiver oil, extracted from the roots of the grass *Vetiveria zizanioides*, gave 2 new tricyclic sesquiterpenoids, zizanal and epizizanal (I; R = CHO, R1 = H; R = H, R1 = CHO) (II and III, resp.) together with the known compds.  $\alpha$ - and  $\beta$ -vetivone, khusimone, and bicyclicodecenone (IV). The structures of II and III were determined by standard chemical and spectral methods. II and III showed insect repelling activity.  
 IT 15764-04-2  
 RL: BIOL (Biological study)  
 (from *Vetiveria zizanioides*)  
 RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d stat que l11

```

L1      33 SEA FILE=REGISTRY ABB=ON  PLU=ON  NOOTKATON?
L2      SEL  PLU=ON  L1 1- CHEM :      100 TERMS
L3      492 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2
L4      492 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3 OR NOOTKATON?
L5      7087 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (TICKS/CV OR ACARI/CV) OR
        TICK OR ACARI OR ANTITICK? OR ANTIACARI?
L6      6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4 AND L5
L7      194193 SEA FILE=HCAPLUS ABB=ON  PLU=ON  PESTICIDES/CV OR ACARICIDES/CV
        OR INSECTICIDES/CV OR RODENTICIDES/CV REPELLENTS/CV OR
        PESTICIDE OR INSECTICIDE OR RODENTICIDE OR REPELLENT
L8      16 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L4 AND L7) NOT L6
L9      4916981 SEA FILE=HCAPLUS ABB=ON  PLU=ON  MATERIAL OR SOIL OR POLYMER?
        OR DIATOMACEO? OR DIATOMITE OR SAND OR CELLULOSE
L10     34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4 (L) L9
L11     28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 NOT (L6 OR L8)

```

=> d ibib abs hitstr l11 1-28

L11 ANSWER 1 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:933468 HCAPLUS  
 DOCUMENT NUMBER: 142:196838  
 TITLE: Determination method for radical-scavenging activities  
 of foods using 1,1-diphenyl-2-picrylhydrazyl, and  
 method for using of authentic compounds as antioxidant  
 Choi, Hyang Sook  
 INVENTOR(S):  
 PATENT ASSIGNEE(S): S. Korea  
 SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given  
 CODEN: KRXXA7  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Korean  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2002037434	A	20020521	KR 2000-67513	20001114
PRIORITY APPLN. INFO.:			KR 2000-67513	20001114

AB Provided are determination method for radical-scavenging activities of foods using 1,1-diphenyl-2-picrylhydrazyl, and method for using of authentic compds. as antioxidant such as alpha terpinene, gamma terpinene, terpinolene, citronellal, citral, geraniol and nootkatone. The free radical scavenger prevents cardiovascular disease, cerebrovascular, cancer and aging by eliminating free radicals from the body. The determination method for radical-scavenging activities of foods comprises adding essential oil, authentic fragrance material, buffer solution, ethanol and

emulsifier to the test sample then adding DPPH thereto; adding a standard antioxidant for the determination of the oxidation resistance to the above mixture and stirring it in a shaker; settling it in the dark at room temperature for 30 min and determining the decrease of the DPPH peak by HPLC at 517nm; and determining the anti-oxidancy of the sample by using the peak height of HPLC according to formula of Trolox equivalency.

L11 ANSWER 2 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:492733 HCAPLUS  
 DOCUMENT NUMBER: 141:53287  
 TITLE: Citrus flavoring materials  
 INVENTOR(S): Kawasaki, Kiyomitsu  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 38 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004168936	A2	20040617	JP 2002-338193	20021121

PRIORITY APPLN. INFO.: JP 2002-338193 20021121

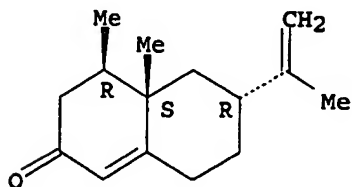
AB The invention relates to citrus flavoring materials suitable for use in food products characterized by containing natural fragrances, esters, alcs., aldehyde, ketones, phenols, ethers, lactones, hydrocarbons, nitrogen-containing and/or sulfur-containing compds., and/or acids. An orange flavoring material composition containing sweet orange oil 70, dodecyl acetate 1, lavandulyl acetate 1, octyl butyrate 0.5, decanal di-Et acetal 1, 10-undecen-1-ol 1, 2,4-dodecadienal 1, nerol oxide 2, and solvent q.s. to 100 % was formulated for making orange juice beverage.

IT 4674-50-4, Nootkatone 5195-69-7  
 RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
 (citrus flavoring materials containing defined components)

RN 4674-50-4 HCAPLUS

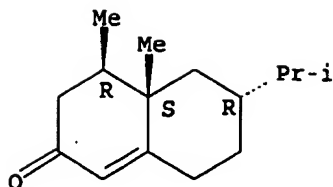
CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 5195-69-7 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 3 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:188726 HCAPLUS  
 DOCUMENT NUMBER: 141:294847  
 TITLE: Monitoring of flavor use in the food industry  
 AUTHOR(S): Pivovarov, Yu. V.; Ivanova, E. V.; Zenin, V. A.  
 CORPORATE SOURCE: FGU "Sergievo-Posadskii TsSM", Russia  
 SOURCE: Pivo i Napitki (2003), (4), 46-49  
 CODEN: PNIABR  
 PUBLISHER: OOO Izdatel'stvo "Pishchevaya Promyshlennost"  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB An overview is given of the applications of gas chromatog. with mass-selective detection for recognizing anomalous or fraudulent flavor components and flavoring materials in food products. Examples discussed include propylene glycol in flavored tea; triacetin in fruit nectar; Et benzoate, Me anthranilate, and di-Me anthranilate in grape juice; menthol derivs. in lemon beer; nootkatone in grapefruit juice; and racemic mixts. of several compds. in pineapple juice.

L11 ANSWER 4 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:178186 HCAPLUS  
 DOCUMENT NUMBER: 140:216522  
 TITLE: Organoleptic agents comprising nootkatone  
 INVENTOR(S): Tamura, Hiroshi; Amaike, Masayasu; Warita, Yasuhiro; Ishikawa, Masashi; Takagi, Keiichi  
 PATENT ASSIGNEE(S): Hasegawa Koryo Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004067723	A2	20040304	JP 2002-224777	20020801
PRIORITY APPLN. INFO.:				
			JP 2002-224777	20020801

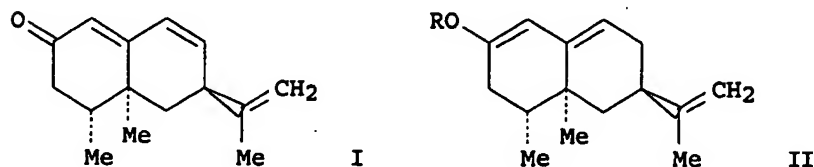
AB This invention relates to flavoring agents containing nootkatone, valencene epoxide, and nootkatol. The compns. provide long-lasting taste and smell-like grapefruit. For example, a flavoring composition was formulated containing grapefruit oil 989, nootkatone 10, valencene epoxide 0.5, and nootkatol 0.5 part. The composition was used for flavoring candies and drinks.

L11 ANSWER 5 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:95650 HCAPLUS  
 DOCUMENT NUMBER: 140:146306  
 TITLE: Preparation of 2-alkoxynootkatene and 8,9-didehydronootkatone for flavoring and fragrant materials

INVENTOR(S): Amano, Akira; Sakaguchi, Tamizo  
 PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004035455	A2	20040205	JP 2002-194171	20020703
PRIORITY APPLN. INFO.:			JP 2002-194171	20020703
OTHER SOURCE(S):	MARPAT 140:146306			

GI



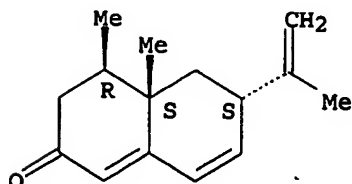
AB 8,9-Didehydronootkatone I is prepared by dehydrogenation-oxidation of 2-alkoxynootkatene II (R = C1-4 alkyl). Optically inactive compound is similarly prepared. Thus, reaction of nootkatone with Et orthoformate in the presence of p-toluenesulfonic acid gave 93% 2-ethoxynootkatene, which was treated with chloranil in aqueous acetone at 20-22° for 5.5 h to afford 91.6% I.

IT 653571-57-4P, (±)-Dehydronootkatone  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (preparation of didehydronootkatone for flavoring and fragrant materials via alkoxynootkatene)

RN 653571-57-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

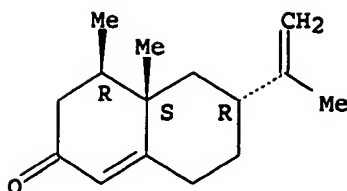


IT 4674-50-4, Nootkatone  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of didehydronootkatone for flavoring and fragrant materials via alkoxynootkatene)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 6 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:702882 HCAPLUS  
 DOCUMENT NUMBER: 139:213017  
 TITLE: Manufacture of nootkatone with Mucor sp.  
 INVENTOR(S): Hashimoto, Toshihiro; Asakawa, Yoshinori; Noma, Yoshiaki; Murakami, Chie; Furusawa, Mai; Kanisawa, Tsuneyoshi; Emura, Makoto; Mitsuhashi, Katsuhisa  
 PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003250591	A2	20030909	JP 2002-51668	20020227
PRIORITY APPLN. INFO.:			JP 2002-51668	20020227

AB Nootkatone (I), useful as a flavoring and perfume material, is manufactured by conversion of valencene (II) into I with Mucor sp. Mucor sp. was shake-cultured in MY medium for 6 days, shake-cultured in Czapek-peptone medium at 27° for 4 days, and cultured in the medium with addition of 100 mg II at 27° for 11 days to give 65.2 mg I (61.0% yield) of ≥95% purity.

L11 ANSWER 7 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:446117 HCAPLUS  
 DOCUMENT NUMBER: 137:19737  
 TITLE: Substituted cyclohexenes as flavoring materials  
 INVENTOR(S): Goeke, Andreas  
 PATENT ASSIGNEE(S): Givaudan SA, Switz.  
 SOURCE: Eur. Pat. Appl., 19 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1213276	A1	20020612	EP 2000-126655	20001205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
WO 2002046131	A1	20020613	WO 2001-EP14107	20011203
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,				

Pryor 10\_769830 Claim 76

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,  
 UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,  
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 AU 2002018322 A5 20020618 AU 2002-18322 20011203  
 EP 1339659 A1 20030903 EP 2001-999545 20011203  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2004515482 T2 20040527 JP 2002-547871 20011203  
 US 2004073050 A1 20040415 US 2003-433342 20030523  
 PRIORITY APPLN. INFO.: EP 2000-126655 A 20001205  
 WO 2001-EP14107 W 20011203

OTHER SOURCE(S): MARPAT 137:19737

AB The present invention relates to substituted cyclohexenes, to their use as well as to their preparation method. These compds. have powerful long lasting natural fruity grapefruit notes with minty and fresh green tonalities and can be used as flavoring materials.

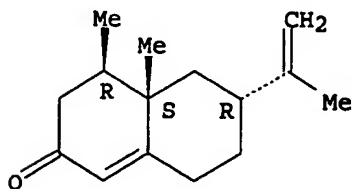
IT 4674-50-4, Nootkatone

RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)  
 (substituted cyclohexenes as flavoring materials)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:31309 HCAPLUS

DOCUMENT NUMBER: 136:101498

TITLE: Use of hydrophilic membranes to obtain flavors and other extracts

INVENTOR(S): Gradley, Michelle Lorraine

PATENT ASSIGNEE(S): Zylepsis Limited, UK

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002213	A1	20020110	WO 2001-GB3003	20010704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,				

Pryor 10\_769830 Claim 76

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,  
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1296752 A1 20030402 EP 2001-945526 20010704  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2004501757 T2 20040122 JP 2002-506833 20010704  
 US 2003185956 A1 20031002 US 2003-312438 20030529  
 PRIORITY APPLN. INFO.: GB 2000-16312 A 20000704  
 WO 2001-GB3003 W 20010704

AB A method for extracting one or more desired components from a mixture in an aqueous

phase comprises separating the aqueous mixture from a water-immiscible hydrophobic phase by means of a hydrophilic membrane and allowing the desired components to move out of the aqueous phase through the membrane and into the hydrophobic phase. The remaining components have a lower water solubility than the desired component(s), such that the remaining components are incapable of passing through the membrane. The method may be used for the isolation of materials from reaction mixts., for purification purposes or for the preparation of exts. of natural substances (flavors and aromas). Thus, selective extraction of nootkatone from grapefruit peel is attained by using a cellulose acetate dialysis membrane. Exts. may be produced in the form of carrier-based flavors, for instance absorbed on paper or maltodextrins, or encapsulated into maltodextrins, including into glass forms; which can then be formed into powders or tablets and used as such.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:678276 HCAPLUS

DOCUMENT NUMBER: 135:299936

TITLE: Effects of nootkatone and a borate compound on formosan subterranean termite (Isoptera: Rhinotermitidae) and its symbiont protozoa

AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.  
 CORPORATE SOURCE: Department of Entomology, Louisiana State University  
 Agricultural Center, Baton Rouge, LA, 70803, USA

SOURCE: Journal of Entomological Science (2001), 36(3), 229-236

CODEN: JESCEP; ISSN: 0749-8004

PUBLISHER: Georgia Entomological Society, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Wood treated with disodium octaborate tetrahydrate, with nootkatone, a natural extract isolated from vetiver oil, or with both nootkatone and disodium octaborate tetrahydrate was tested for effects on *Coptotermes formosanus* Shiraki and its hindgut flagellates. After 7 d disodium octaborate tetrahydrate-treated wood induced high termite mortality and almost complete loss of flagellates, confirming the toxicity of borates to these termites. Wood treated with nootkatone alone or with the nootkatone-borate mix was consumed in significantly lower amts. than the control, and termite survival was comparable to results obtained for starved termites. A significant progressive reduction in the total number of protozoa was observed for all groups, including the controls. Thus, nootkatone acts as a

feeding deterrent, inducing starvation that results in almost a complete loss of *Pseudotrichonympha grassii*, the most important flagellate species for cellulose digestion in this termite.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:290022 HCAPLUS  
DOCUMENT NUMBER: 134:312041  
TITLE: Apparatus for chemically compacting styrene polymer foams  
INVENTOR(S): Sakai, Tokue  
PATENT ASSIGNEE(S): Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001114927	A2	20010424	JP 1999-299017	19991021
PRIORITY APPLN. INFO.:			JP 1999-299017	19991021

AB The apparatus, useful for recycling styrene polymer foam wastes, comprises a main container part for dissolving the foam wastes in solvents (nootkatone, limonene, etc.), a lid having a device for pushing the foam wastes in the solvents, and a ring seal having a groove to fit the edge of the lid or the container, wherein the lid or the container has a groove on the edge to place the seal. Solvent leaking when the seal is swollen by the solvents is prevented with this apparatus. An illustration of the apparatus is given.

L11 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:178386 HCAPLUS  
DOCUMENT NUMBER: 134:221521  
TITLE: Process for the preparation of nootkatone by laccase catalysis  
INVENTOR(S): Huang, Rongmin; Christenson, Philip A.; Labuda, Ivica M.  
PATENT ASSIGNEE(S): Givaudan S.A., Switz.  
SOURCE: U.S., 14 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6200786	B1	20010313	US 1999-391785	19990908
ZA 2000004379	A	20010228	ZA 2000-4379	20000824
EP 1083233	A1	20010314	EP 2000-117432	20000828
EP 1083233	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 247715	E	20030915	AT 2000-117432	20000828
AU 739171	B2	20011004	AU 2000-53700	20000829
SG 87164	A1	20020319	SG 2000-4972	20000831
BR 2000004038	A	20010522	BR 2000-4038	20000906

CA 2317893 AA 20010308 CA 2000-2317893 20000907  
 JP 2001103989 A2 20010417 JP 2000-270975 20000907  
 PRIORITY APPLN. INFO.: US 1999-391785 A 19990908  
 OTHER SOURCE(S): CASREACT 134:221521  
 AB A method of producing nootkatone by laccase catalyzed oxidation of valencene. Valencene and microorganisms such as Botrytis cinerea or Trametes versicolor, which have laccase activity, are reacted in the presence of an oxygen source, at a valencene concentration greater than 0.1%, to form valencene hydroperoxide. The valencene hydroperoxide is then degraded to nootkatone by ether heating or by reaction with a catalyst such as iron, ascorbic acid, cobalt, copper or any combination of these catalysts. In an alternative embodiment, a purified or partially purified laccase of microbial origin may be employed to produce valencene hydroperoxide. Optionally, a mediator and/or a solvent at a concentration that maintains laccase activity may also be included. Such mediators include: 1-hydroxybenzotriazole, 2,2'-azino-bis(3-ethylbenzthiazolene-6-sulfonic acid), ferulic acid, dimethoxy benzyl alc., dimethylaminobenzoic acid, catechin, epicatechin, p-hydroxyphenylacetic acid, quercetin, chlorpromazine, phenothiazine, naringin, promazine, homovanillic acid, 4-amino-salicylic acid, syringic acid, 4-hydroxycinnamic acid, 4-amino-3-hydroxybenzoic acid, vanillic acid, isovanillic acid, caffeic acid,  $\alpha$ -resorcylic acid,  $\beta$ -resorcylic acid,  $\gamma$ -resorcylic acid, 2,3-dihydroxybenzoic acid, 3,4-dihydroxybenzoic acid, 4-hydroxybenzoic acid, 3-hydroxybenzoic acid, 2,4,6 trihydroxybenzoic acid, benzoic acid, cinnamic acid, sodium benzoate, salicylic acid or combinations of these mediators. The enzymic conversion may be conducted with orange oil or other citrus essential oils that contain valencene. The method produces nootkatone in com. viable yields. Thus, a reaction mixture consisting of 60 nkat/mL laccase from Botrytis cinerea, 0.5% Tween 80, 0.5 mM 1-hydroxybenzotriazole, and 0.5% valencene was incubated in a shake flask at 30 °C at pH 3.5 for six days with a resulting nootkatone yield of 59.1%.  
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2001:50714 HCAPLUS  
 DOCUMENT NUMBER: 134:116793  
 TITLE: Volume-reducing agent for polystyrene foams  
 INVENTOR(S): Katsuta, Kimio  
 PATENT ASSIGNEE(S): Bio Venture Bank Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 12 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004192	A1	20010118	WO 2000-JP4704	20000713
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

JP 1999-199522

A 19990713

AB The convenient environmentally friendly volume-reducing agent is obtained by adding to a solvent (e.g., nootkatone-containing grapefruit peel extract) for polystyrene foams an insolubilizing agent (e.g., EtOH, hexane) in which polystyrene foams are insol. but which is soluble in the solvent for polystyrene foams. Upon contact with the volume-reducing agent, a polystyrene foam becomes a curdy matter floating thereon without dissolving in the volume-reducing agent. By cleansing the curdy matter, a raw polystyrene material can be obtained from which a polystyrene foam can be regenerated.

REFERENCE COUNT:

15

THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:871784 HCAPLUS

DOCUMENT NUMBER: 134:105588

TITLE: Nootkatone

AUTHOR(S): Letizia, C. S.; Cocchiara, J.; Wellington, G. A.;  
Funk, C.; Api, A. M.

CORPORATE SOURCE: Research Institute for Fragrance Materials, Inc.,  
Hackensack, NJ, 07601, USA

SOURCE: Food and Chemical Toxicology (2000), 38(Suppl. 3),  
S165-S167

CODEN: FCTOD7; ISSN: 0278-6915

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB International Fragrance association has published a guideline recommending that nootkatone used as a fragrance ingredient should be at least 98% pure with a m.p. of at least 32°. Lower-purity nootkatone, with a min. purity of 86% should not exceed a level of 1% and should be used only in conjunction with at least 4-fold the amount of d-limonene. Nootkatone was given Generally Recognized As Safe status as a flavor ingredient by Flavor and Extract Manufacturers' Association and approved for food use by FDA.

IT 4674-50-4, Nootkatone

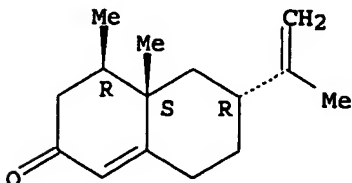
RL: BUU (Biological use, unclassified); FFD (Food or feed use); BIOL (Biological study); USES (Uses)

(nootkatone as fragrance material and flavoring agent for food)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:335465 HCAPLUS  
 DOCUMENT NUMBER: 132:322708  
 TITLE: Nootkatone or nootkatone analog derivatives and their use as solvents for recycling or compacting of styrene plastics  
 INVENTOR(S): Kashihara, Hiroshi  
 PATENT ASSIGNEE(S): Kukita, Takeshi, Japan  
 SOURCE: PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000027907	A1	20000518	WO 1999-JP6228	19991109
W: AU, BR, CA, CN, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2001131111	A2	20010515	JP 2000-32103	20000209
PRIORITY APPLN. INFO.:			JP 1998-335003	A 19981110
			WO 1999-JP6228	A 19991109

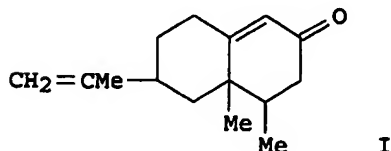
OTHER SOURCE(S): MARPAT 132:322708

AB Grapefruit peel extract and nootkatone (or its analogs) and nootkatone (or its analog) derivs. are used in volume-reduction, dissoln. and recycling of plastic foams (hydrocarbon polymer plastics such as polystyrene and polypropylene), eliminating oily stains, dissoln. of cholesterol, etc. Compared with D-limonene, these substances can reduce the volume of a large amount of plastics (styrene foam, etc.) even in a small amount. Moreover, the resultant solns. containing plastics (styrene foam, etc.) dissolved therein can be easily post-treated at low temps. In addition, nootkatone (or its analogs) contained in grapefruit extract can be converted into nootkatone (or its analog) derivs. by chemical treatments and these derivs. show similar effects.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 15 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:610355 HCAPLUS  
 DOCUMENT NUMBER: 113:210355  
 TITLE: Essential oil composition of different grapefruit varieties  
 AUTHOR(S): Abkhazava, D. M.; Kharebava, L. G.  
 CORPORATE SOURCE: VNIICHSKICH P, USSR  
 SOURCE: Subtropicheskie Kul'tury (1989), (6), 111-16  
 CODEN: SUKUA8; ISSN: 0491-4031  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB Forty-eight compds. were isolated, of which 38 were identified, in oils of different grapefruit varieties. The major compound was limonene comprising 67.60-88.09%, while nootkatone (I), the compound which gives a characteristic aroma of grapefruit, comprised 0.1-0.35% of the oil. The oil yields were 8.3-33.7 µg/g raw material.

L11 ANSWER 16 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:572378 HCAPLUS

DOCUMENT NUMBER: 113:172378

TITLE: Reaction products of geranonitrile and dihydrolinalool with thioacetic acid and their use as aroma or taste enhancers

INVENTOR(S): Boden, Richard M.; McGhie, Joseph A.

PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA

SOURCE: Eur. Pat. Appl., 146 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

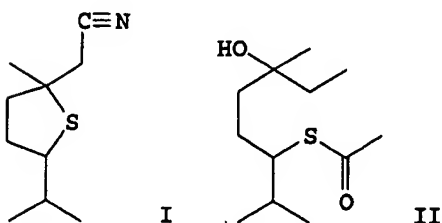
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 369668	A2	19900523	EP 1989-311552	19891108
EP 369668	A3	19900926		
R: CH, DE, FR, GB, LI, NL				
US 4883884	A	19891128	US 1988-273016	19881118
US 4886897	A	19891212	US 1988-273017	19881118
US 4962089	A	19901009	US 1989-424601	19891020
PRIORITY APPLN. INFO.:			US 1988-273016	A 19881118
			US 1988-273017	A 19881118
			US 1989-424601	A 19891020

GI



AB Sixteen products of the reaction of AcSH with geranonitrile (a mixture of isomeric nitriles Me<sub>2</sub>C:CHCH<sub>2</sub>CH:CMech<sub>2</sub>CN and Me<sub>2</sub>C:CHCH<sub>2</sub>CH<sub>2</sub>CMe:CHCN) and with dihydrolinalool Me<sub>2</sub>C:CMech<sub>2</sub>CH<sub>2</sub>C(OH)MeCH<sub>2</sub>Me, especially a thiophene derivative I

and a thioacetate II, useful for augmenting or enhancing the aroma or taste of consumable materials, perfume compns., and detergents, were prepared Thus, AcSH was added dropwise to geranonitrile at 64° over 60 min and the mixture was stirred 1 h at 65-70° and 1.5 h at 70-75° to give I which had a natural buchu leaf, tomato leaf, herbaceous, basil, minty, and grapefruit-like aroma from a fragrance standpoint, and a green, minty, grapefruit-like and nootkatone-like aroma and taste profile. Scented polyethylene and polypropylene pellets, a deodorant stick and liquid detergent composition, a grapefruit flavor,

chewing gum, and toothpaste formulations, etc. containing I were prepared

L11 ANSWER 17 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:552461 HCAPLUS  
DOCUMENT NUMBER: 111:152461  
TITLE: Commercially processed orange juice products having a more hand-squeezed character  
INVENTOR(S): Swaine, Robert L., Jr.; Rich, Thomas F.; Strobel, Rudolf G. K.; Thundathil, Raju V.; Tsai, Chee Hway  
PATENT ASSIGNEE(S): Procter and Gamble Co., USA  
SOURCE: Eur. Pat. Appl., 50 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

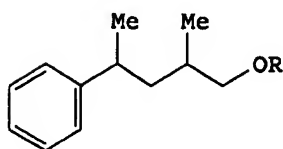
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 292047	A2	19881123	EP 1988-200908	19880509
EP 292047	A3	19910306		
EP 292047	B1	19930908		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 94031	E	19930915	AT 1988-200908	19880509
ES 2058234	T3	19941101	ES 1988-200908	19880509
CA 1332535	A1	19941018	CA 1988-566638	19880512
JP 01055166	A2	19890302	JP 1988-121639	19880518
PRIORITY APPLN. INFO.:			US 1987-52088	A 19870518
			EP 1988-200908	A 19880509

AB Com. processed orange juice products, including frozen orange juice concs., which are closer to handsqueezed orange juice in character, are disclosed. At single-strength, these products have a viscosity of  $\leq 7$  cP (at 8°) and a titratable oil content of  $\leq 0.015\%$ . These products are further characterized by an orange aroma and flavor component which has a higher ratio of certain desirable "fresh" and "orangey" compds., relative to certain less desirable orange compds., when compared to current com. orange juice products prepared from orange juice concentrate. The ratio of the combined amount of acetaldehyde, Et butyrate, Et 3-hydroxyhexanoate and valencene to the combined amount of hexanal,  $\alpha$ -pinene, myrcene, decanal, linalool, octanol, 4-terpineol,  $\alpha$ -terpineol, dodecanal, and nootkatone is  $\geq 2:1$ . Carefully-selected fruits are gently extracted to provide a juice having  $\leq 0.015$ , preferably 0.010% titratable peel oil. Finishing of the juice is carried out by removing the nonjuice materials and the "sensible" pulp.

L11 ANSWER 18 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1987:72732 HCAPLUS  
DOCUMENT NUMBER: 106:72732  
TITLE: Uses of 2-methyl-4-phenyl-1-pentanol derivatives in augmenting or enhancing the aroma or taste of consumable materials  
INVENTOR(S): Hall, John B.  
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA  
SOURCE: U.S., 26 pp. Division of U.S. Ser. No. 681,656.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4610812	A	19860909	US 1985-784059	19851004
US 4650898	A	19870317	US 1984-681656	19841214
PRIORITY APPLN. INFO.: GI			US 1984-681656	A3 19841214



AB Pentanol derivs. I (R = H, Ac) are added to consumable materials, e.g. perfume compns., colognes, perfumed articles, foodstuffs, chewing gums, medicinal products, and chewing tobacco, to augment or enhance the aroma or taste. I (R = H) has a powerful long-lasting stable green grapefruit-like, nootkatone-like, animalic, leathery, vetiver-like, olibanum, musky and floral aroma profile; and a floral, green, weedy, fruity, grapefruit, galbanum-like aroma and taste at 1 ppm. I (R = Ac) has a green, styrallyl acetate-like aroma; and a floral, nootkatone-like, oriental, green pepper-like aroma and taste at 1 ppm. I (R = H) was prepared by condensation of propanal with hydratropic aldehyde to give a mixture containing isomeric 2-methyl-4-pentenals, which were hydrogenated using Raney Ni catalyst. I (R = H) was acetylated with Ac2O in presence of concentrate H3PO4 to give I (R = Ac). A herbal perfume formulation contained Oakmoss absolute 20, 2-methyl-3,4-(methylenedioxy)hydrocinnamic aldehyde 10, Me dihydrojasmonate 100 coumarin 20, musk ketone 80, isocyclocitral 10, galbanum oil 6 rosemary oil 10, pine needle oil 60, fir balsam absolute 10, bergamot oil 60, lemon oil 14, benzyl acetate 468, linalool 80, indole 6, undecalactone 12 and I (R = H) 12 parts by weight

L11 ANSWER 19 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1985:23234 HCAPLUS  
 DOCUMENT NUMBER: 102:23234  
 TITLE: Citrus juice concentrate  
 INVENTOR(S): Powers, John Robert; Moore, Robert Sidney; Anderson, Barry Jay; Downton, Galen Edward; Kennedy, Judith Ann; Kearney, Donald Raymond; Strang, David Arthur  
 PATENT ASSIGNEE(S): Procter and Gamble Co., USA  
 SOURCE: Eur. Pat. Appl., 59 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 110638	A2	19840613	EP 1983-307049	19831118
EP 110638	A3	19860409		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
NO 8304218	A	19840521	NO 1983-4218	19831117
NO 158444	B	19880606		

Pryor 10\_769830 Claim 76

NO 158444	C	19880914		
FI 8304238	A	19840520	FI 1983-4238	19831118
FI 78381	B	19890428		
FI 78381	C	19890810		
JP 59146562	A2	19840822	JP 1983-217625	19831118
CA 1213167	A1	19861028	CA 1983-441439	19831118
CA 1213168	A1	19861028	CA 1983-441491	19831118
CA 1213169	A1	19861028	CA 1983-441492	19831118
PRIORITY APPLN. INFO.:			US 1982-443083	A 19821119
			US 1983-504922	A 19830616
			US 1983-504924	A 19830616
			US 1983-505012	A 19830616

AB An orange juice concentrate containing 60% of the volatiles naturally occurring in the juice and 33% of the solids (pulp, sugars, pectin) is produced. Thus, volatiles were steam stripped from orange juice at 37.7-71° and ≤9 in. of Hg, condensed (at 32° to -196° depending on pressure) into oil (limonene [5989-27-5]) and aqueous essence fractions, concentrated, and added back (at >2% of the final product) to the juice concentrate obtained by evaporation. The volatile fractions may also be added back to a carrier for use as a flavorant for beverages, candy, etc. The process may be applied in the production of other citrus juice concs. The composition of citrus volatile fractions is given.

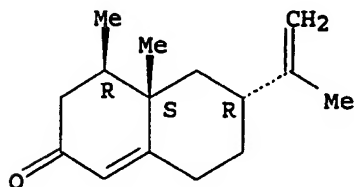
IT 4674-50-4

RL: BIOL (Biological study)  
(of citrus, in flavoring material and concentrated citrus juice manufacture)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 20 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:550196 HCAPLUS

DOCUMENT NUMBER: 101:150196

TITLE: Dehydronootkatone as a perfumery and flavoring ingredient

INVENTOR(S): Demole, Edouard Paul; Enggist, Paul

PATENT ASSIGNEE(S): Firmenich S. A., Switz.

SOURCE: Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----

Pryor 10\_769830 Claim 76

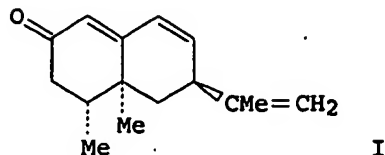
EP 110034	A2	19840613	EP 1983-109130	19830915
EP 110034	A3	19850403		
EP 110034	B1	19861210		

R: CH, DE, FR, GB, LI

PRIORITY APPLN. INFO.:  
GI

CH 1982-6361

A 19821102



AB Dehydronootkatone (I) [5090-63-1] is useful as a perfumery and flavoring ingredient for fruit juices. Thus, I was evaluated for its organoleptic properties. A syrup, prepared from sucrose (650 g) and water 1 L containing 0.25% citric acid, was mixed with 5 ppm I. The drink thus obtained had a fruity and flowery character and resembled the note of grapefruit.

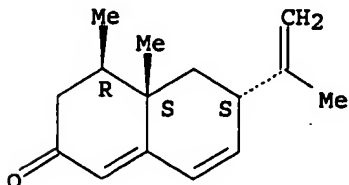
IT 5090-63-1

RL: BIOL (Biological study)  
(perfume and flavoring material)

RN 5090-63-1 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4 $\alpha$ ,4a $\alpha$ ,6 $\beta$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 21 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:495775 HCAPLUS

DOCUMENT NUMBER: 95:95775

TITLE: Use of 1,3,5,5,-tetramethyl-2-2-oxabicyclo[2.2.2.]octane in augmenting or enhancing the aroma or taste of foods

INVENTOR(S): Sprecker, Mark A.; Schmitt, Frederick L.; Vock, Manfred H.; Vinals, Joaquin F.; Kiwala, Jacob  
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA  
SOURCE: U.S., 21 pp. Cont.-in-part of U.S. 4,195,099.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

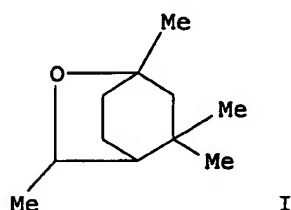
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4269862	A	19810526	US 1979-77539	19790921

Pryor 10\_769830 Claim 76

US 4195099	A	19800325	US 1978-953128	19781020
US 4203947	A	19800520	US 1979-8925	19790202
US 4283576	A	19810811	US 1979-100528	19791205
US 4267067	A	19810512	US 1980-176093	19800807
US 4289705	A	19810915	US 1980-176050	19800807
US 4303725	A	19811201	US 1980-176092	19800807
US 4320771	A	19820323	US 1980-176112	19800807
PRIORITY APPLN. INFO.:			US 1978-953128	A2 19781020
			US 1977-850845	A3 19771111
			US 1979-8925	A3 19790202
			US 1979-52334	A3 19790627
			US 1979-77539	A3 19790921

GI



AB 1,3,5,5-Tetramethyl-2-oxabicyclo[2.2.2]octane (I) [78474-70-1] is prepared and used to give a fresh or minty flavor to food, tobacco, pharmaceuticals, and other products. Thus, mesityl oxide [141-79-7] in a suspension of  $\text{AlCl}_3$  in MePh was reacted with isoprene [78-79-5] to yield 4-acetyl-1,3,3-trimethyl-1-cyclohexene [55695-36-8]. The latter was reduced with  $\text{NaBH}_3$  to give 1,3,3-trimethyl-1-cyclohexene-4-ethanol [78474-71-2] which was reacted with iso-PrOH [67-63-0] and  $\text{H}_2\text{SO}_4$  to yield I. A eucalyptus oil flavor formulation showed more natural eucalyptus flavor as well as a pleasant citrus nuance and sour effect when I was included at 200 ppm.

IT 4674-50-4

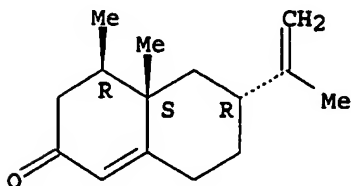
RL: BIOL (Biological study)

(flavoring material containing tetramethyloxabicyclooctane and)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



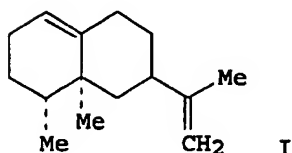
L11 ANSWER 22 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:460079 HCAPLUS

DOCUMENT NUMBER: 85:60079

TITLE: Juvenile hormone activity of some sesquiterpenes of essential oil of orange

AUTHOR(S): Primo Yufera, E.; Tadeo Lluch, J. L.; Ribo Canut, J.; Sendra Sena, J.  
 CORPORATE SOURCE: Inst. Agroquim. Tecnol. Aliment., Valencia, Spain  
 SOURCE: Revista de Agroquimica y Tecnologia de Alimentos (1976), 16(1), 69-78  
 CODEN: RATLAB; ISSN: 0034-7698  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Spanish  
 GI



AB Five sesquiterpenes of orange oil ( $\alpha$ -copaene,  $\beta$ -elemene, caryophyllene, valencene (I), and  $\delta$ -cadinene and some oxygenated derivs. of I (nootkatone, epoxy nootkatone, and epoxy I) were tested on pupae of *Triboleum castaneum* to determination juvenile hormone activity and on ovaries of *Blattella germanica* to determination gonadotropic hormone activity. A weak activity was observed for some sesquiterpenes, particularly the oxygenated derivs. of I. Some sesquiterpene structures may be suitable starting materials for the synthesis of new hormonomimetics.

L11 ANSWER 23 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1974:569645 HCAPLUS  
 DOCUMENT NUMBER: 81:169645  
 TITLE: Microbiological study of terpenes. Valencene  
 AUTHOR(S): Dhavlikar, R. S.; Albroscheit, G.  
 CORPORATE SOURCE: Forschungslab., Dragoco, Holzminden, Fed. Rep. Ger.  
 SOURCE: Dragoco Report (German Edition) (1974), 20(12), 251-8  
 CODEN: DRGRAV; ISSN: 0366-9645  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Valencene fermentation by bacteria from Dutch soil and inoculated domestic beer in a mineral salt medium gave 7.5% epoxide I, 8%  $\alpha$ -cyperone (II), 18% ketone III, and 18% nootkatone (IV), identified by chemical and spectroscopic methods.

L11 ANSWER 24 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1971:63285 HCAPLUS  
 DOCUMENT NUMBER: 74:63285  
 TITLE: Odor character and threshold values of nootkatone and related compounds  
 AUTHOR(S): Stevens, Kenneth L.; Guadagni, Dante G.; Stern, Donald J.  
 CORPORATE SOURCE: West. Util. Res. Dev. Div., U. S. Dep. Agric., Albany, CA, USA  
 SOURCE: Journal of the Science of Food and Agriculture (1970), 21(11), 590-3

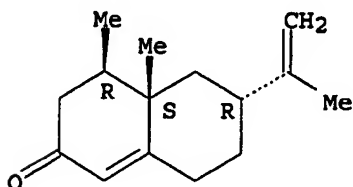
CODEN: JSFAAE; ISSN: 0022-5142  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The odor character and potency of nootkatone obtained from grapefruit oil were compared with those of some closely related compds. These compds. may differ considerably in qual. but the potency remains similar. In addition, synthesized racemic nootkatone had the same potency as the naturally occurring material.

L11 ANSWER 25 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1968:458428 HCAPLUS  
DOCUMENT NUMBER: 69:58428  
TITLE: Food additives. Synthetic flavoring substances and adjuvats  
AUTHOR(S): Anon.  
SOURCE: Federal Register (1968), 33(144), 10569, 25 Jul 1968  
CODEN: FEREAC; ISSN: 0097-6326  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The following addnl. flavoring substances are added to the list of materials that may be used in food under the Federal Food, Drug, and Cosmetic Act: linalool oxide [cis- and trans-2-vinyl-2-methyl-5-(1-hydroxy-1-methylethyl)tetrahydrofuran]; methadienol [p-mentha-1,8(10)-dien-9-ol]; methadienyl acetate [p-mentha-1,8(10)-dien-9-yl acetate]; nootkatone (5,6-dimethyl-8-isopropenylbicyclo[4.4.0]-dec-1-en-3-one); ocimene (trans- $\beta$ -ocimene; 3,7-dimethyl-1,3,6-octatriene); perillaldehyde (4-isopropenyl-1-cyclohexane-1-carboxaldehyde; p-mentha-1,8-dien-7-al); perillyl acetate (p-mentha-1,8-dien-7-yl acetate).

IT 4674-50-4  
RL: BIOL (Biological study)  
(as flavoring material and food additive)

RN 4674-50-4 HCAPLUS  
CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 26 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1967:402248 HCAPLUS  
DOCUMENT NUMBER: 67:2248  
TITLE: Flavor studies of nootkatone in grapefruit juice  
AUTHOR(S): Berry, Robert E.; Wagner, Charles J., Jr.; Moshonas, M. G.  
CORPORATE SOURCE: U.S. Dep. of Agr., Southern Util. Res. and Develop. Div., Winter Haven, FL, USA  
SOURCE: Journal of Food Science (1967), 32(1), 75-8  
CODEN: JFDSAZ; ISSN: 0022-1147  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A study was made to determine the flavor threshold of nootkatone (I) in grapefruit juice, and to determine the level at which I would be beneficial. Samples examined in water and (or) reconstituted crystals were: natural I separated from grapefruit peel oil, synthetic I purified once by gas chromatog., synthetic I purified several times by gas chromatog., and crystalline I. I could be detected at 1 ppm. in water, and at 6 ppm. in 10.5° Brix reconstituted juice. All 4 I samples had the same flavor threshold. A I level of 6-7 ppm. was generally considered desirable, but at a level >7 ppm., some judges rated the product as bitter.

IT 4674-50-4

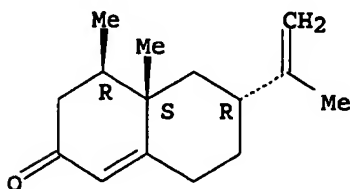
RL: BIOL (Biological study)

(as flavoring material in grapefruit juice)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 27 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1966:19565 HCAPLUS

DOCUMENT NUMBER: 64:19565

ORIGINAL REFERENCE NO.: 64:3610b-d

TITLE: Conversion of valencene to nootkatone

AUTHOR(S): Hunter, G. L. K.; Brogden, W. B., Jr.

CORPORATE SOURCE: U.S. Dept. of Agr., Winter Haven, FL

SOURCE: Journal of Food Science (1965), 30(5), 876-8

CODEN: JFDSA; ISSN: 0022-1147

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Orange condensate oil (5 gal.) was separated from the vapors removed from orange juice during com. orange concentrate preparation The oil was distilled at

80° 1 mm. to remove most of the limonene. The residue (450 ml.) was distilled to give 1st 150 ml. limonene, and then 200 ml. valencene (I). O-containing materials were removed by percolation through basic Al<sub>2</sub>O<sub>3</sub>, with hexane as eluant. The solvent was removed, and I obtained by rectification in a spinning band column at 108°, 5 mm. Hg. tert-Bu chromate reagent was prepared by treating tert-BuOH with CrO<sub>3</sub>. Treatment of I in CCl<sub>4</sub>-AcOH-(AcO)<sub>2</sub>O with the tert-Bu chromate reagent 45 min. at 50° and then 22 hrs. at 60°, followed by cooling, dilution with H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> solution, and extraction with CCl<sub>4</sub>, gave an extract of nootkatone (II). This extract was washed with water and with K<sub>2</sub>CO<sub>3</sub> solution, and dried over Na<sub>2</sub>SO<sub>4</sub> to give a 67% yield of II.

L11 ANSWER 28 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1961:22923 HCAPLUS

DOCUMENT NUMBER: 55:22923

ORIGINAL REFERENCE NO.: 55:4572b-i

TITLE: Terpenes. CXV. Stereoisomeric vetivanes and sesquiterpenic hydrocarbons of vetiver oil

AUTHOR(S): Romanuk, M.; Herout, V.

CORPORATE SOURCE: Ceskoslov. akad. ved, Prague

SOURCE: Collection of Czechoslovak Chemical Communications (1960), 25, 2540-52  
CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. *ibid.* 1837. Saponification of vetiver oil (Ia) (256 g.,  $d_{20} 0.9975$ ,  $n_{20D} 1.5234$ ) with 100 mL. 7.5% alc. KOH 1 h. and extraction with Et<sub>2</sub>O gave 214.1 g. nonsapond. material, which on treatment with Girard reagent P followed by purification via semicarbazones afforded 175 mg.  $\alpha$ -vetivone (I),  $d_{20} 0.9996$ ,  $n_{20D} 1.5315$ ; semicarbazone m. 210° (decomposition),  $[\alpha]_{20D} 306^\circ$ , and 290 mg.  $\beta$ -vetivone (II),  $d_{20} 0.9950$ ,  $n_{20D} 1.5320$ ; semicarbazone m. 227° (decomposition),  $[\alpha]_{20D} -69.4^\circ$ . Hydrogenation of I (170 mg.) in 25 mL. MeOH over 500 mg. 5% Pd-SrCO<sub>3</sub> gave 162 mg.  $\alpha$ -vetivanone (tetrahydro- $\alpha$ -vetivone) (III), b<sub>2.5</sub> 139-41°,  $n_{20D} 1.4861$ ; semicarbazone m. 225°. Treatment of 140 mg. III with 300 mg. (CH<sub>2</sub>SH)<sub>2</sub> and 300 mg. BF<sub>3</sub>·Et<sub>2</sub>O in 3 mL. AcOH 1 h. at room temperature gave 182 mg. ethylene thioketal of III (IIIa), m. 77° (petr. ether). Refluxing 170 mg. IIIa with 5 mL. Raney Ni in 20 mL. dioxane 16 h. and extracting with pentane gave vetivane (IV), C<sub>15</sub>H<sub>28</sub>, b<sub>16</sub> 128°,  $d_{20} 0.8849$ ,  $n_{20D} 1.4714$ . Hydrogenation of 220 mg. II over 40 mg. PtO<sub>2</sub> in 6 mL. AcOH and chromatog. on 2.5 g. Al<sub>2</sub>O<sub>3</sub> gave, by petr. ether elution, 15.3 mg. isovetivane (V), b<sub>20</sub> 125-30°,  $d_{20} 0.8840$ ,  $n_{20D} 1.4720$ , and by elution with 1:1 Et<sub>2</sub>O-MeOH, 150 mg.  $\beta$ -vetivanol, m. 100-2° (petr. ether) whose oxidation with CrO<sub>3</sub> in 60% AcOH 24 h. at room temperature afforded  $\beta$ -vetivanone (tetrahydro- $\beta$ -vetivone) (VI), b<sub>1</sub> 142°,  $n_{20D} 1.4852$ ; semicarbazone m. 199°. Treatment of 40 mg. VI with (CH<sub>2</sub>SH)<sub>2</sub> and Raney Ni gave 19 mg. V. Hydrogenation of 150 mg. vetivazulene over 50 mg. PtO<sub>2</sub> in AcOH gave 125 mg. decahydrovetivazulene (VII), b<sub>12</sub> 120-3°,  $d_{20} 0.8820$ ,  $n_{20D} 1.4782$ , probably a mixture of stereoisomers C<sub>15</sub>H<sub>28</sub> with prevailing trans junction of the rings. Distillation of the residue after the removal of the acids and ketones from 410.5 g. Ia, chromatog. of the 78.2 g. fraction b. at 110-30°/10 mm. over Al<sub>2</sub>O<sub>3</sub>, elution with petr. ether and distillation of the 56.1 g. residue over a 70 TP column followed by repeated chromatog. over Al<sub>2</sub>O<sub>3</sub> gave: tricyclovetivene C<sub>15</sub>H<sub>24</sub> (VIII),  $d_{20} 0.9395$ ,  $n_{20D} 1.5069$ ,  $[\alpha]_{20D} 37.3^\circ$  [hydrogenation over PtO<sub>2</sub> in AcOH gave dihydrotricyclovetivene (IX), b<sub>15</sub> 124-6°,  $d_{20} 0.9198$ ,  $n_{20D} 1.4951$ ]; 450 mg.  $\alpha$ -isovetivenene (X),  $d_{20} 0.9257$ ,  $n_{20D} 1.5222$ ,  $[\alpha]_{20D} -120.4^\circ$  (hydrogenation over PtO<sub>2</sub> in AcOH afforded hexahydro- $\alpha$ -isovetivenene, b<sub>14</sub> 125-9°,  $d_{20} 0.8853$ ,  $n_{20D} 1.4732$ ); 425 mg. zizanene (XI), C<sub>15</sub>H<sub>24</sub>,  $d_{20} 0.9163$ ,  $n_{20D} 1.5090$   $[\alpha]_{20D} 68.5^\circ$ ; [hydrogenation over PtO<sub>2</sub> in AcOH afforded tetrahydrozizanene (XII), b<sub>12</sub> 122-5°,  $d_{20} 0.8887$ ;  $n_{20D} 1.4811$ ]; 0.41 g.  $\beta$ -isovetivenene (XIII), C<sub>15</sub>H<sub>22</sub>,  $d_{20} 0.9268$ ,  $n_{20D} 1.5235$ ,  $[\alpha]_{20D} -68.4^\circ$ ; (hexahydro- $\beta$ -isovetivenene or V,  $d_{20} 0.8815$ ,  $n_{20D} 1.4763$ );  $\alpha$ -vetivenene (XIV), C<sub>15</sub>H<sub>22</sub> (0.21 g.)  $d_{20} 0.9308$ ,  $n_{20D} 1.5152$ ,  $[\alpha]_{20D} 142.4^\circ$ ; (hexahydrovetivenene or IV, b<sub>15</sub> 126-9°,  $d_{20} 0.8914$ ,  $n_{20D} 1.4765$ );  $\beta$ -vetivenene (XV), C<sub>15</sub>H<sub>22</sub> (0.81 g.),  $d_{20} 0.9469$ ,  $n_{20D} 1.5378$   $[\alpha]_{20D} -192.6^\circ$ ; and 0.24 g. dehydrovetivenene, C<sub>15</sub>H<sub>20</sub>,  $d_{20} 0.9501$ ,  $n_{20D} 1.5518$ ,  $[\alpha]_{20D} 176.7^\circ$ ; octahydrodehydrovetivenene (IR spectrum similar to IV), C<sub>15</sub>H<sub>28</sub>, b<sub>16</sub> 128-30°,  $d_{20} 0.9034$ ,  $n_{20D} 1.4760$ . IR spectra of I-VII and X-XV were given.

=> => d stat que 116

L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?  
 L2 SEL PLU=ON L1 1- CHEM : 100 TERMS  
 L3 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L2  
 L4 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L3 OR NOOTKATON?  
 L5 7087 SEA FILE=HCAPLUS ABB=ON PLU=ON (TICKS/CV OR ACARI/CV) OR  
 TICK OR ACARI OR ANTITICK? OR ANTIACARI?  
 L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND L5  
 L7 194193 SEA FILE=HCAPLUS ABB=ON PLU=ON PESTICIDES/CV OR ACARICIDES/CV  
 OR INSECTICIDES/CV OR RODENTICIDES/CV REPELLENTS/CV OR  
 PESTICIDE OR INSECTICIDE OR RODENTICIDE OR REPELLENT  
 L8 16 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND L7) NOT L6  
 L9 4916981 SEA FILE=HCAPLUS ABB=ON PLU=ON MATERIAL OR SOIL OR POLYMER?  
 OR DIATOMACEO? OR DIATOMITE OR SAND OR CELLULOSE  
 L10 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L4(L) L9  
 L11 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT (L6 OR L8)  
 L15 42 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4(L) (TREAT? OR APPLY OR  
 APPLIED)) NOT (L6 OR L8)  
 L16 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L11

=> d ibib abs hitstr 116 1-37

L16 ANSWER 1 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1261357 HCAPLUS  
 DOCUMENT NUMBER: 144:652  
 TITLE: Autonomic nerve-modulating agents containing terpenes  
 INVENTOR(S): Kagawa, Taiji  
 PATENT ASSIGNEE(S): Kao Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

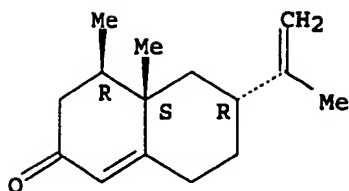
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005330208	A2	20051202	JP 2004-148981	20040519
PRIORITY APPLN. INFO.:			JP 2004-148981	20040519

AB Title agents, useful for treatment of autonomic imbalance, contain  
 monoterpene alcs., sesquiterpene ketones, and/or diterpene alcs. as active  
 ingredients. Thus, inhalation of germacrone or hinokitiol to lower  
 respiratory tract increased or decreased heart rate, resp., in rats.

IT 4674-50-4, Nootkatone  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (autonomic nerve-modulating agents containing terpenes for  
 treatment of autonomic imbalance)

RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:186982 HCAPLUS

TITLE: Development and testing of new insecticidal wood preservatives

AUTHOR(S): Henderson, Gregg; Smith, W. Ramsay; Laine, Roger A.

CORPORATE SOURCE: Department of Entomology, LSU AgCenter, Baton Rouge, LA, 70803-1710, USA

SOURCE: Abstracts of Papers, 229th ACS National Meeting, San Diego, CA, United States, March 13-17, 2005 (2005), CELL-157. American Chemical Society: Washington, D. C.

CODEN: 69GQMP

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB The move away from metal-based and highly toxic wood preservatives has begun with the shift from arsenicals in the USA and copper-based products in Europe. The future appears to lie in natural and natural-based products. A better understanding of insect biol. as it relates to insecticidal wood preservatives and new preservative designs are helping to develop new treatments. The history of insecticidal chemistries has gone through several generations of development including heavy metals, organophosphates, borates and organo copper, nicotine and pyrethrum derivs., fipronil, combinations of single compds. with boron, performance additives, and newer natural and natural-based products including nootkatone, 2-acetonaphthone, and plant-derived oils. New treatment methods for engineered wood products and testing methodologies and a new method of extraction of wood preservatives for quality control purposes will be presented.

L16 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:609329 HCAPLUS

DOCUMENT NUMBER: 141:145397

TITLE: Production of perfume compositions for incorporation to strong alkali preparations

INVENTOR(S): Oguro, Daichi; Okubo, Yasutaka; Warita, Yasuhiro;

Omori, Yoshihiro; Matsui, Masanao

PATENT ASSIGNEE(S): Hasegawa Koryo Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004211054	A2	20040729	JP 2003-180586	20030625
PRIORITY APPLN. INFO.:			JP 2002-330454	A 20021114

AB Perfume compns. comprising alcs., aldehydes, and/or ketones are treated

with acidic ion exchangers to be incorporated to bleaches and hair dye compns. containing strong alkali oxidants. For example, a perfume composition containing tetrahydrolinalool 10.5, undecylenic aldehyde 0.1, lauric aldehyde 0.2,  $\alpha$ -damascone 0.2, geraniol 20, phenylethyl alc. 25, hexylcinnamic aldehyde 5, Me dihydrojasmonate 15, liral 10, Me cedryl ketone 10, and heliotropine 4 %. The perfume composition 40, ethanol 20, and Diaion SK 1B 2 g were mixed at .apprx. 80° for 5 h, cooled, and the ion exchanger was separated out. The composition was washed with a saline solution,

dried using MgSO<sub>4</sub>, and added to a hair dye composition

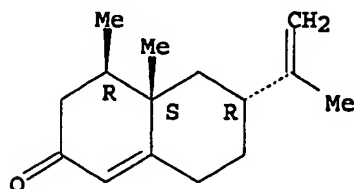
IT 4674-50-4, Nootkatone

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(acidic ion exchanger-treated perfume compns. for  
incorporation to bleaches and hair dyes)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:884528 HCAPLUS

DOCUMENT NUMBER: 139:381632

TITLE: Preparation of organic compounds using cyclic imide catalysts

INVENTOR(S): Kitayama, Kenji; Sekiguchi, Kazuya

PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

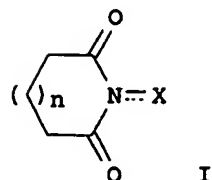
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003321413	A2	20031111	JP 2002-125417	20020426
PRIORITY APPLN. INFO.:			JP 2002-125417	20020426
OTHER SOURCE(S):			MARPAT 139:381632	

GI



AB Organic compds. are prepared by treatment of organic substrates with catalysts having cyclic imide skeletons I (n = 0, 1; X = O, OR; R = H, protective group), wherein oxidation inhibitors are preliminary removed from the substrates by oxidation or column chromatog. Valencene was treated with MnO<sub>2</sub> and oxidized by O in the presence of N-hydroxyphthalimide, Co acetate, Co acetylacetonate, and Co(NO<sub>3</sub>)<sub>2</sub> in MeCN to give 62% **nootkatone**.

L16 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:531810 HCAPLUS  
DOCUMENT NUMBER: 137:231677  
TITLE: Use of **nootkatone** as a senescence indicator for Rouge La Toma Cv. Grapefruit (Citrus paradisi Macf.)  
AUTHOR(S): Biolatto, Andrea; Sancho, Ana M.; Cantet, Rodolfo J. C.; Guéemes, Daniel R.; Pensel, Norma A.  
CORPORATE SOURCE: Instituto Tecnologia de Alimentos Centro de Agroindustrias, Instituto Nacional de Tecnologia Agropecuaria INTA, Buenos Aires, Argent.  
SOURCE: Journal of Agricultural and Food Chemistry (2002), 50(17), 4816-4819  
CODEN: JAFCAU; ISSN: 0021-8561  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The objective of this research was to study the usefulness of **nootkatone** as a senescence indicator for Rouge La Toma cv. grapefruit (Citrus paradisi Macf.), simulating different treatments that included the normal postharvest handling of citrus fruits: temperature conditioning, cold storage, shipment periods to overseas markets such as Japan and the U.S., marketing conditions, and storage at nonchilling temperature (control treatments). The highest **nootkatone** levels, determined by GLC-MS analyses, were detected in fruits subjected to control treatments. No significant differences were observed in **nootkatone** levels between treatments either with or without temperature conditioning prior to the start of the cold storage. Levels of **nootkatone** increased throughout time for all assayed treatments. The linear regressions of **nootkatone** levels showed correlation coeffs. of 0.80 and 0.83 with storage time (29 and 42 days, resp.). Therefore, **nootkatone** appears to be a good indicator of senescence for Rouge La Toma grapefruit.

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:113150 HCAPLUS  
DOCUMENT NUMBER: 136:167527  
TITLE: Isolation of **nootkatone** by inclusion reaction  
INVENTOR(S): Kanehata, Akiko; Akiyama, Takeshi; Nakajima, Kazuomi  
PATENT ASSIGNEE(S): Yasuhara Chemical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

JP 2002047239 A2 20020212 JP 2000-269400 20000802  
 PRIORITY APPLN. INFO.: JP 2000-269400 20000802

AB Nootkatone (I) is isolated its mixts. by treatment with cyclic compds. for selective formation of inclusion complexes and releasing I from the complexes. An orange oil fraction was treated with hydroxypropyl-β-cyclodextrin to give I of 79.8% purity with .apprx.80% recovery.

L16 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:932488 HCAPLUS

DOCUMENT NUMBER: 136:53914

TITLE: Preparation of conjugated unsaturated carbonyl compounds with imides and cobalt salt catalysts under mild conditions

INVENTOR(S): Kitayama, Kenji

PATENT ASSIGNEE(S): Daicel Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

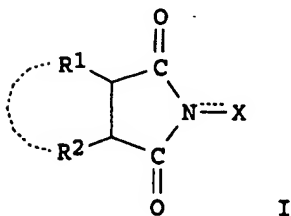
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001354611	A2	20011225	JP 2000-176494	20000613
PRIORITY APPLN. INFO.:			JP 2000-176494	20000613
OTHER SOURCE(S):	CASREACT 136:53914; MARPAT 136:53914			

GI



AB Conjugated unsatd. carbonyl compds., useful as fragrant substances, etc., are prepared by introduction of oxo group to CH<sub>2</sub> group adjacent to C-C double bond in the presence of imides I [R<sub>1</sub>, R<sub>2</sub> = H, halo, alkyl, aryl, cycloalkyl, OH, alkoxy, etc.; R<sub>1</sub>R<sub>2</sub> may form (N-substituted imide group-containing) double bond, (aromatic) ring; X = O, OH] and Co(II) salts with acids with pK<sub>a</sub> ≤ 8.0 as catalysts. Thus, valencene was treated with N-hydroxyphthalimide, (AcO)<sub>2</sub>Co·4H<sub>2</sub>O, and Co(III) acetylacetonate under O at 40° for 2 h in MeCN to give 58% nootkatone.

L16 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:890707 HCAPLUS

DOCUMENT NUMBER: 134:114988

TITLE: Classification and analysis of citrus oils by NIR spectroscopy

AUTHOR(S): Steuer, B.; Schulz, H.; Lager, E.

CORPORATE SOURCE: Federal Centre for Breeding Research on Cultivated  
Plants, Institute for Quality Analysis, Quedlinburg,  
D-06484, Germany  
SOURCE: Food Chemistry (2000), Volume Date 2001, 72(1),  
113-117  
CODEN: FOCHDJ; ISSN: 0308-8146  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A new NIRS method is introduced for the determination of valuable components in various citrus oils. Spectra of grapefruit, orange, mandarin, lemon and lime oils in the range from 1100 to 2500 nm have been registered. Applying principal component anal. to the spectral data a good separation of the different fruit oil types can be achieved. The application of multivariate statistics in conjunction with anal. reference data leads to good NIR calibration results. For the main components (e.g. limonene,  $\gamma$ -terpinene, sabinene) and general chemical-phys. parameters (e.g. optical rotation value, aldehyde content) standard errors are in the range of the applied reference method. The multiple coeffs. of determination (R<sup>2</sup>) for components with an amount of more than 1.5% are generally >0.95. Furthermore reliable in-process methods for the determination of the individual nootkatone and aldehyde contents during the isolation and purification process from grapefruit and orange oil are presented.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:321456 HCAPLUS  
DOCUMENT NUMBER: 132:352791  
TITLE: Pharmaceutical suppository composites for fever and influenza and method of producing the composites  
INVENTOR(S): Hsu, Wu-ching; Keng, Su-hsien  
PATENT ASSIGNEE(S): Taiwan  
SOURCE: U.S., 17 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6063383	A	20000516	US 1999-238744	19990128
PRIORITY APPLN. INFO.:			US 1999-238744	19990128

AB Pharmaceutical suppository composites for fever and influenza and a method of producing them are disclosed. More particularly, the composites combine all the advantages of traditional Chinese medicine, Western medicine, and phys. temperature reduction to relieve symptoms of influenza. Poisonous side effects can be avoided by using the disclosed suppositories. The pharmaceutical suppository composites comprise 2750-3250 g radix bupleuri scorzonrifolium wild, 1750-2250 g flos lonicerae japonicae, 1950-2450 g fructus forsythiae, 1650-2150 g fructus arctii, 2550-3050 g herba schizonepetae, 50-550 g calculus bovis, and 870-1370 g of excipients.

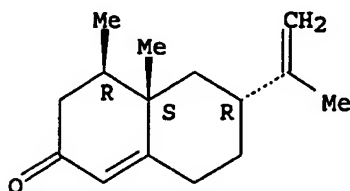
IT 4674-50-4

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)  
(suppositories containing exts. of Chinese medicines for treatment of fever and influenza)

RN 4674-50-4 HCAPLUS

CN 2 (3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:138471 HCAPLUS

TITLE: Flavor impact components of grapefruit juice: Processing and maturity changes.

AUTHOR(S): Jella, P.; Rouseff, R.; Goodner, K.

CORPORATE SOURCE: Citrus Research and Education Center, University Florida, Lake Alfred, FL, 33850-2299, USA

SOURCE: Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), AGFD-004. American Chemical Society: Washington, D. C. CODEN: 65QTAA

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

AB Twenty-four flavor impact components were quantified in 40 com. not-from-concentrate grapefruit juices using sulfur chemiluminescence, flame ionization, GC-olfactometry (OSME or CHARM), HPLC and GC/MS/MS. Effect of temperature and time-temperature was determined using pasteurized and unpasteurized (early, mid and late season) juices. Aroma activity decreased due to pasteurization. Increased fruity attributes were observed in late season juices when compared to early season juices. Several aroma components were lost due to thermal processing. Total number and total areas of sulfur peaks decreased with increasing fruit maturity. Heat treatment appeared to have aroma impact. One of these peaks has been identified as p-menthene-8-thiol and the other is yet to be identified. Myrcene,  $\beta$ -caryophyllene and linalool were found to differentiate between juices of various flavor preference while nootkatone was relatively ineffective in differentiating the preference classes. Identifications in addition to qual. and quant. changes in the aroma active components will be presented.

L16 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:520920 HCAPLUS

DOCUMENT NUMBER: 127:202922

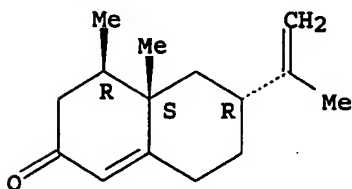
TITLE: Aromatic plants of tropical Central Africa. XXVIII. Influence of cultural treatment and harvest time on vetiver oil quality in Burundi

AUTHOR(S): Dethier, M.; Sakubu, S.; Ciza, A.; Cordier, Y.; Menut, C.; Lamaty, G.

CORPORATE SOURCE: Laboratoire de Technologie, Faculte des Sciences Agronomiques de l'Universite du Burundi, Bujumbura, Burundi

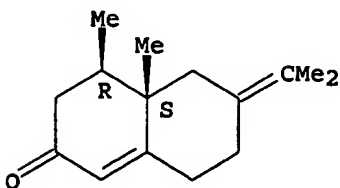
SOURCE: Journal of Essential Oil Research (1997), 9(4), 447-451  
 CODEN: JEOREG; ISSN: 1041-2905  
 PUBLISHER: Allured  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Vetiver (*Vetiveria zizanioides* (Stapf.)) is grown in Burundi for its anti-erosive properties. A study to determine the effects of organic manure or a combination of organic manure and NPK fertilizer was performed. Criteria such as root yield, effect on harvest time, oil yield, oil quality and composition were examined. It was found that soil treatments increased the root yield from 1,500 kg/ha to ca 2,400 kg/ha, while harvest time effected oil quality and yield. Also the khusimol content ranged from 19.4-29.5%, and some oils were judged as having superior quality.  
 IT 4674-50-4, Nootkatone 15764-04-2,  $\alpha$ -Vetivone  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)  
 (influence of cultural treatment and harvest time on vetiver oil quality in Burundi)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1993:597692 HCAPLUS  
 DOCUMENT NUMBER: 119:197692  
 TITLE: Influence of ethylene and ethephon on the sesquiterpene nootkatone production in *Citrus paradisi*  
 AUTHOR(S): Ortuno Tomas, A.; Garcia-Puig, D.; Sabater, F.;

CORPORATE SOURCE: Porras, I.; Garcia-Lidon, A.; Del Rio, J. A.  
 SOURCE: Fac. Biol., Univ. Murcia, Murcia, 30071, Spain  
 Journal of Agricultural and Food Chemistry (1993),  
 41(10), 1566-9  
 CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The effect of ethylene and ethephon treatments on  
 nootkatone accumulation in the rind of grapefruit was  
 investigated. Considerable increases in the levels of this sesquiterpene  
 were observed in the picked and unpicked grapefruits treated. The  
 changes induced in the maturation-senescence stage of grapefruit by these  
 treatments consisted of an accelerated carotenogenesis process in  
 the rind, along with morphol. changes in the exocarp and ultrastructural  
 changes in the plastids. Thus, ethylene regulates nootkatone  
 biosynthesis by accelerating the maturation-senescence processes in  
 grapefruit rind.

L16 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:517591 HCAPLUS  
 DOCUMENT NUMBER: 117:117591  
 TITLE: Deodorant for indoor air treatment  
 INVENTOR(S): Mizobuchi, Manabu; Yamauchi, Toshiyuki; Shoji, Shiho  
 PATENT ASSIGNEE(S): Matsushita Electric Works, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF

DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

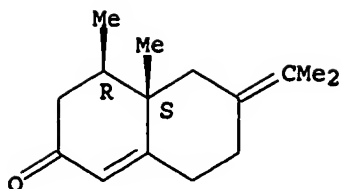
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04030857	A2	19920203	JP 1990-139378	19900528
PRIORITY APPLN. INFO.:			JP 1990-139378	19900528

AB A deodorant for removing NH<sub>3</sub>, amines, and H<sub>2</sub>S from odorous air in toilets,  
 kitchens, and closed rooms is prepared from plant exts. mainly containing  
 ≥1 compound selected from menthone, cineol, geraniol, vetiverol,  
 vetiverone, β-vetivone, vetivene, 1-menthol, citronellol, 1-linalool,  
 linalyl acetate, 2-terpineol, and dipentene. Thus, a Forsythia suspensa  
 extract containing 1-linalool, linalyl acetate, and dipentene was dispersed in  
 an  
 ETOH solution to give a formulated deodorant for removing NH<sub>3</sub> and Me  
 mercaptan from odorous air in a closed container.

IT 15764-04-2  
 RL: OCCU (Occurrence)  
 (plant extract containing, for deodorant preparation, for indoor air  
 treatment)

RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L16 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1991:663037 HCAPLUS  
 DOCUMENT NUMBER: 115:263037  
 TITLE: Volatile constituents of several varieties of pummelos and characteristics among citrus species  
 AUTHOR(S): Sawamura, Masayoshi; Shichiri, Kenichi; Ootani, Yoshitaka; Zheng, Xiao Hong  
 CORPORATE SOURCE: Fac. Agric., Kochi Univ., Kochi, 783, Japan  
 SOURCE: Agricultural and Biological Chemistry (1991), 55(10), 2571-8  
 CODEN: ABCHA6; ISSN: 0002-1369  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Cold-pressed oil (CPO) components from 8 varieties of pummelos were identified and measured.  $\gamma$ -Terpinene was the second major component in 4 varieties, but only a minor component in the others. Cadina-1(10), 6,8-triene was identified by GC-MS in addition to the 63 compds. identified already. Multivariate analyses were applied to 37 kinds of citrus fruits including pummelos and other species. The pummelo was classified into 2 groups by cluster anal., and into 3 groups by principal component anal. on the basis of the oxygenated composition (wt/wt%) in fresh CPOs. The tendency for classification agreed in the two analyses. Nootkatone was the only discriminating component of the pummelo species from others. The results are also discussed in citrus species other than pummelo, being compared with the botanical classifications.

L16 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1990:134455 HCAPLUS  
 DOCUMENT NUMBER: 112:134455  
 TITLE: Effect of gibberellic acid and 2-(3,4-dichlorophenoxy)triethylamine on nootkatone in grapefruit peel oil and total peel oil content  
 AUTHOR(S): Wilson, Charles W., III; Shaw, Philip E.; McDonald, Roy E.; Greany, Patrick D.; Yokoyama, Henry  
 CORPORATE SOURCE: U. S. Citrus Subtrop. Prod. Lab., Winter Haven, FL, 33883-1909, USA  
 SOURCE: Journal of Agricultural and Food Chemistry (1990), 38(3), 656-9  
 CODEN: JAFCAU; ISSN: 0021-8561  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The nootkatone content in grapefruit peel oil extracted from flavedo and the peel oil content of fruit receiving preharvest treatment with 20 or 50 ppm gibberellic acid (GA) and/or 50, 125, or 250 ppm 2-(3,4-dichlorophenoxy)triethylamine (DCPTA) were determined. Treatment by GA reduced the rate of increase in nootkatone concentration observed in control fruit with maturation, and the effect was dose-dependent. When DCPTA was used alone as the growth regulator, nootkatone content increased significantly. When 50 ppm GA followed DCPTA treatment

at the 3 levels used above, the effect of GA predominated and nootkatone content was significantly lower than that found in untreated fruit. Treatment by GA generally increased peel oil concentration

L16 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1989:39216 HCAPLUS  
 DOCUMENT NUMBER: 110:39216  
 TITLE: Preparation of 7,8-didehydronootkatone  
 INVENTOR(S): Masuda, Hideki; Kikui, Hiromi  
 PATENT ASSIGNEE(S): Ogawa and Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

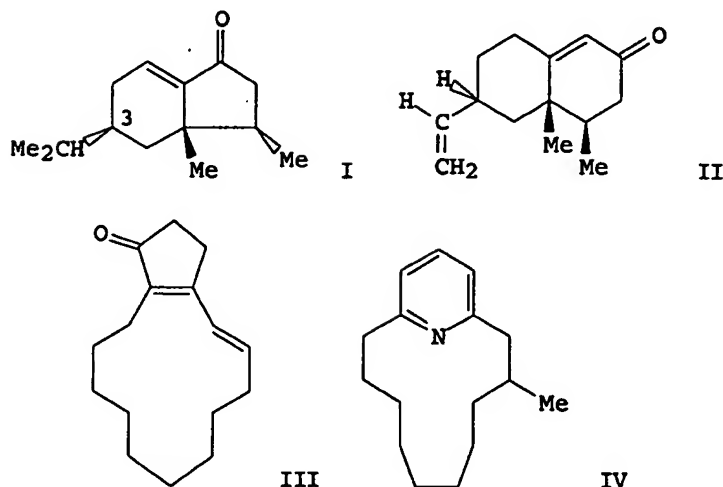
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63162647	A2	19880706	JP 1986-308395	19861226
PRIORITY APPLN. INFO.:			JP 1986-308395	19861226

AB Title compound (I), which is a component of flavor of grapefruit and useful as a flavorant for foods and cosmetics (no data), is prepared by oxidative dehydrogenation of nootkatone (II) with 1-1.5 mol equiv chloranil in nonpolar aprotic organic solvents in such a way that .apprx.20% unreacted II exist in the reaction mixts. II (12 g) was treated with 14 g chloranil in MePh at 90° for .apprx.1 h to give 3.5 g 80:20% mixture of I and II, vs. 87:13% mixture of II and 7,8-didehydro-.alpha.-vetivone when AcOEt was used instead of MePh.

L16 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1983:177816 HCAPLUS  
 DOCUMENT NUMBER: 98:177816  
 TITLE: Direct analysis of food aromas  
 AUTHOR(S): Labows, John N.; Shushan, Bori  
 CORPORATE SOURCE: Monell Chem. Senses Cent., Philadelphia, PA, USA  
 SOURCE: American Laboratory (Shelton, CT, United States) (1983), 15(3), 56-61  
 CODEN: ALBYBL; ISSN: 0044-7749  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A technique, based on the direct introduction of sample vapors into an atmospheric pressure chemical ionization inlet of a mass spectrometer and using 2 mass spectrometers in tandem, with the 1st mass spectrometer for separation of the volatiles and the 2nd for elucidation of their structure, was successfully applied to determination of volatile substances in fruit and sausages. The detectability limits of representative volatiles were 0.5 ppb for Et butyrate, 0.78 ppb for linalool, and 44 ppb for limonene [138-86-3]. In the 4 types of sausages analyzed, the major volatile compds. were EtOH [64-17-5] (teewurst), ProH [62309-51-7] (Westphalian sausage), terpenes, alcs., and esters (salami), and Me2CO [67-64-1] and alcs. (knockwurst). The major volatile compds. of bananas were esters, HOAc [64-19-7], and isoamyl acetate [123-92-2]. Citrus fruits (mangoes, oranges, limes, and lemons) showed the presence of monoterpenes such as limonene and pinene [80-56-8], monoterpene aldehydes such as citral [5392-40-5], and monoterpene alcs. such as terpineol [8000-41-7]. nootkatone [4674-50-4] Was an important flavor compound for grapefruits and oranges.

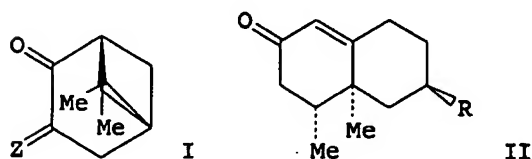
L16 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1982:69232 HCAPLUS  
 DOCUMENT NUMBER: 96:69232  
 TITLE: Regio- and stereoselective cyclopentannulation with ketones and propargyl alcohol derivatives. Synthesis of dl-nootkatone and dl-muscovydine  
 AUTHOR(S): Hiyama, Tamejiro; Shinoda, Masaki; Saimoto, Hiroyuki; Nozaki, Hitosi  
 CORPORATE SOURCE: Dep. Ind. Chem., Kyoto Univ., Kyoto, 606, Japan  
 SOURCE: Bulletin of the Chemical Society of Japan (1981), 54(9), 2747-58  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 96:69232  
 GI



AB A highly regio- and stereoselective five-membered ring annulation involving the acid-treatment of propargyl alc. dianion adducts of ketones is described. The propargyl alc. adduct of 2-octanone was converted into 2-methyl-3-pentyl-2-cyclopentenone by treatment with sulfuric acid-methanol at 0°. As the major product, 1-methylbicyclo[5.3.0]dec-6-en-8-one was produced from 2-methylcycloheptanone. Remarkable regioselective cyclopentannulation was observed in 2-methylcyclohexanone and 2,3-dimethylcyclohexanone wherein 1-methyl- and trans-1,2-dimethyl-substituted bicyclo[4.3.0]non-5-en-7-one (BNO) are produced, resp. With 3-butyne-2-ol, 2-methylcyclohexanone was converted into cis-1,9-dimethyl-substituted BNO. 4-Isopropyl-2-methylcyclohexanone was transformed into a mixture of isopropylbicyclononone I and its 3 epimer. These results are explained in terms of the conrotatory ring-closure of thermodynamically most favorable hydroxypentadienyl cation intermediates. 3-Methoxycarbonyl-cis-1,9-dimethyl-BNO produced from 4-methoxycarbonyl-2-methylcyclohexanone and 3-butyne-2-ol was successfully transformed into dl-nootkatone (II) by converting the methoxycarbonyl group into isopropenyl of correct stereochem. followed by ring enlargement. Cyclopentannulation using propargyl alc. dianion adducts of 2-cycloalkenones is discussed.

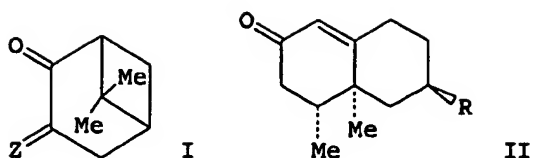
Annulation takes place regioselectively to give conjugated dienones, e.g., bicyclopentadecadienone III from 2-cyclododecenone. This product is led to dl-muscovydine IV by conjugate 1,6-addition of Me group followed by ring expansion and finally by aromatization with HONH<sub>2</sub>.HCl.

L16 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1980:198554 HCAPLUS  
 DOCUMENT NUMBER: 92:198554  
 TITLE: Highly efficient synthesis of (+)-nootkatone from (-)-β-pinene  
 AUTHOR(S): Miyashita, Masaaki; Yanami, Tetsuji; Yoshikoshi, Akira  
 CORPORATE SOURCE: Chem. Res. Inst. Non-Aqueous Solutions, Tohoku Univ., Sendai, Japan  
 SOURCE: Koen Yoshishu - Tennen Yuki Kagobutsu Toronkai, 22nd (1979), 190-7. Kyushu Univ., Fac. Sci., Dep. Chem.: Fukuoka, Japan.  
 CODEN: 42MAAQ  
 DOCUMENT TYPE: Conference  
 LANGUAGE: Japanese  
 GI



AB trans-3-Ethylidenenopinone [I, Z = (E)-MeCH], obtained by condensation of I (Z = H<sub>2</sub>) with MeCHO, was treated with CH<sub>2</sub>:CHCH<sub>2</sub>SiMe<sub>3</sub> in the presence of TiCl<sub>4</sub> to give the methylbutenyl derivative I (Z = α-H, β-CH<sub>2</sub>:CHCH<sub>2</sub>CHMe), which was methylated with MeI in the presence of NaNH<sub>2</sub> to give I (Z = α-Me, β-CH<sub>2</sub>:CHCH<sub>2</sub>CHMe), whose oxidation with Hg(OAc)<sub>2</sub> gave I (Z = α-Me, β-MeCOCH<sub>2</sub>CHMe). Cyclization of the diketone in AcOH-HCl gave the (chloroisopropyl)naphthalenone II (R = CMe<sub>2</sub>Cl), which was dehydrochlorinated to give nootkatone (II, R = CMe:CH<sub>2</sub>) in 72% yield.

L16 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1980:129117 HCAPLUS  
 DOCUMENT NUMBER: 92:129117  
 TITLE: Synthetic study of (+)-nootkatone from (-)-β-pinene  
 AUTHOR(S): Yanami, Tetsuji; Miyashita, Masaaki; Yoshikoshi, Akira  
 CORPORATE SOURCE: Chem. Res. Inst. Non-Aqueous Solutions, Tohoku Univ., Sendai, 980, Japan  
 SOURCE: Journal of Organic Chemistry (1980), 45(4), 607-12  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Condensing (+)-nopinone with MeCHO followed by acid treatment gave ethylidenenopinone I (Z = MeCH) whose treatment with CH<sub>2</sub>:CMeCH<sub>2</sub>SiMe<sub>3</sub> gave I (Z = α-H, β-CH<sub>2</sub>:CMeCH<sub>2</sub>CHMe). The last was methylated with MeI-NaNH<sub>2</sub> to give I (Z = α-Me, β-CH<sub>2</sub>:CMeCH<sub>2</sub>CHMe) whose ozonolysis gave I [Z = α-Me, β-(R)-MeCOCH<sub>2</sub>CHMe], reaction of which with HCl gave naphthalenone II (R = CMe<sub>2</sub>Cl), whose dehydrochlorination over Al<sub>2</sub>O<sub>3</sub> gave (±)-nootkatone II (R = CMe:CH<sub>2</sub>).

L16 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:537301 HCAPLUS

DOCUMENT NUMBER: 79:137301

TITLE: Stereoselective approach to eremophilane sesquiterpenes. Synthesis of (+-)-nootkatone Dastur, K. P.

AUTHOR(S): Res. Sch. Chem., Aust. Natl. Univ., Canberra, Australia

SOURCE: Journal of the American Chemical Society (1973), 95(19), 6509-10

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The bicyclic derivative (I, R = CO<sub>2</sub>Me), obtained by Diels-Alder reaction of the cyclohexadiene (II) with MeO<sub>2</sub>CCH:CH<sub>2</sub> followed by SeO<sub>2</sub> oxidation and Wittig reaction, was treated with MeLi in Et<sub>2</sub>O at room temperature to give I (R = CMe<sub>2</sub>OH), which in the presence of HCO<sub>2</sub>H gave the naphthalene derivative (III, R = CMe<sub>2</sub>O<sub>2</sub>CH). Refluxing the latter collidine 15 hr in the presence of neutral alumina gave 75% nootkatone (III, R = CMe:CH<sub>2</sub>).

L16 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:72677 HCAPLUS

DOCUMENT NUMBER: 76:72677

TITLE: Eremophilane sesquiterpene derivatives

PATENT ASSIGNEE(S): N. V. Chemische Fabriek "Naarden"

SOURCE: Ger. Offen., 25 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2130184	A	19711223	DE 1971-2130184	19710615
NL 7009040	A	19711221	NL 1970-9040	19700619
CH 566954	A	19750930	CH 1971-8960	19710618
US 3835192	A	19740910	US 1971-154960	19710621
PRIORITY APPLN. INFO.:			NL 1970-9040	A 19700619

AB Optically active sesquiterpenes of the nootkatane series were prepared from 2-methylsabenaketone via 5,6-dimethyl-8-isopropyltricyclo[4.4.0.0<sup>8,10</sup>]dec-1-en-3-one (I). Thus 2-methylsabenaketone was treated with NaNH<sub>2</sub>, the NH<sub>3</sub> boiled off, and then treated with trans-3-penten-2-one at -20° to give 67.5% I. Treatment of 1 g I with 10 ml 1:1 96% H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O gave 0.6 g 5,6 - dimethyl -8-isopropylbicyclo [4.4.0]deca -1,9 - dien - 3 - one. When HCl-EtOH was used to treat I 7-chloro-8,9-dihydronootkatone was obtained, which was used to prepare some related compds., including 11-chloro-8,9-dihydronootkatone, 11-hydroxy-8,9-dihydronootkatone, and . alpha.-vetivone.

L16 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:402795 HCAPLUS  
DOCUMENT NUMBER: 73:2795  
TITLE: Aldehydes, ketones, and esters in Valencia orange peel oil  
AUTHOR(S): Moshonas, Manuel G.; Lund, Eric D.  
CORPORATE SOURCE: Southern Util. Res. and Develop. Div., Agr. Res. Serv., Winter Haven, FL, USA  
SOURCE: Journal of Food Science (1969), 34(6), 502-3  
CODEN: JFDSA2; ISSN: 0022-1147  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB A technique previously employed (Hunter, et al., 1965) was applied to the separation and identification of Valencia orange oil compds. It involved distillation of the oil into several cuts, followed by fractionation of

each cut on a neutral alumina column, and finally gas-liquid chromatog. anal. of the fractions from the column. The following compds. were detected: hexanal, heptanal, octanal, 6-methyl-5-hepten-2-one, nonanal, trans- and cis-limonene oxide, octyl acetate, citronellal, decanal, undecanal, neral, geranial, dodecanal, carvone, perillyl acetate, perillaldehyde, p-metha-1,8-dien-9-yl acetate, piperitenone, nootkatone, α- and β-sinensal, and 5 unidentified aldehydes.

L16 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:121729 HCAPLUS  
DOCUMENT NUMBER: 72:121729  
TITLE: Structure of nardostachone  
AUTHOR(S): Pinder, Albert R.  
CORPORATE SOURCE: Dep. of Chem., Clemson Univ., Clemson, SC, USA  
SOURCE: Tetrahedron Letters (1970), (6), 413-15  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s); see printed CA Issue.

AB The structure I was tentatively assigned to (+)-nardostachone (semicarbazone decomposed 230-2°) by spectral and chemical evidence. (+)-Nootkatone (II) treated with (Ph<sub>3</sub>P)3RhCl gave 11,12-dihydronootkatone which upon reaction with N-bromosuccinimide in CCl<sub>4</sub> yielded II i. III dehydrobrominated by heating with γ-collidine gave IV, semicarbazone decomposed 213°. The structure IV was earlier erroneously assigned to nardostachone (Sastry, S. D. et al., 1967).

L16 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:502047 HCAPLUS  
DOCUMENT NUMBER: 71:102047

TITLE: Terpenoids. XV.  $\alpha$ -vetivone  
 AUTHOR(S): Endo, Katsuya; De Mayo, Paul  
 CORPORATE SOURCE: Univ. Western Ontario, London, ON, Can.  
 SOURCE: Chemical & Pharmaceutical Bulletin (1969), 17(7),  
 1324-31  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 71:102047  
 GI For diagram(s), see printed CA Issue.  
 AB The structure of  $\alpha$ -vetivone (I) one of the major  
 odoriferous principles of vetiver oil was reexamd. Air oxidation of I in the  
 presence of N tert-BuOK yielded, after treatment with  
 p-toluenesulfonic acid, a conjugated dienedione. The enantiomeric compound  
 was prepared by oxidation, of the structurally well-established eremophilone,  
 thus requiring that the structure of I be described as shown. Some  
 interesting observations were made with regards O.R.D. and circular  
 dichroism measurements in comparison with curves obtained from  
 cholest-4-en-3-one. Biogenetic relations between some related compds. are  
 also discussed.

L16 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1969:481558 HCAPLUS  
 DOCUMENT NUMBER: 71:81558  
 TITLE: Absolute stereochemistry of ishwarone  
 AUTHOR(S): Govindachari, Tuticorin R.; Nagarajan, K.;  
 Parthasarathy, P. C.  
 CORPORATE SOURCE: Res. Center, C.I.B.A., Bombay, India  
 SOURCE: Journal of the Chemical Society [Section] D: Chemical  
 Communications (1969), (14), 823  
 CODEN: CCJDAO; ISSN: 0577-6171  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB The structures I and II for ishwarone and isoishwarone, resp., were  
 confirmed from chemical data. The ethylene acetal of I, m. 82-4°, was  
 treated with NaBH<sub>4</sub> and then with alkaline H<sub>2</sub>O<sub>2</sub> to give the ethylene  
 acetal of III, m. 105-8°, which was deacetylated to III, m.  
 172-4°. Retroaldol reaction of III, followed by treatment  
 with KOH in HOCH<sub>2</sub>CH<sub>2</sub>OH gave (+)-nootkatone.

L16 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1969:78180 HCAPLUS  
 DOCUMENT NUMBER: 70:78180  
 TITLE: Terpenes CIC. Structure of valerianol, a  
 sesquiterpenic alcohol of the eremophilane type from  
 valerian oil  
 AUTHOR(S): Jommi, Giancarlo; Krepinisky, J.; Herout, Vlastimil;  
 Sorm, Frantisek  
 CORPORATE SOURCE: Univ. Milano, Milan, Italy  
 SOURCE: Collection of Czechoslovak Chemical Communications  
 (1969), 34(2), 593-600  
 CODEN: CCCCCK; ISSN: 0010-0765  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB Valerianol (I), occurring in Valeriana officinalis, shows the same  
 stereochemistry as valencene,  $\alpha$ -vetivone,  
 nootkatone, and nootkatene. Crude I was converted to  
 3,5-dinitrobenzoate, m. 148° (hexane), and this, in turn, decomposed

by refluxing with alc. KOH to yield pure I, n<sub>20</sub>D 1.5117, [α]<sub>20</sub>D 134° (CHCl<sub>3</sub>). Dehydrogenation of I with Se at 340-50° afforded eudalene (picrate m. 91-2°), and oxidation of I with OsO<sub>4</sub> in pyridine-Et<sub>2</sub>O gave II, m. 149-50°, [α]<sub>20</sub>D 32.6° (CHCl<sub>3</sub>). Hydrogenation of I over Adams catalyst in AcOH gave dihydrovalerianol, while dehydration with POCl<sub>3</sub> or SOCl<sub>2</sub> in pyridine yielded a mixture of III, d<sub>20</sub> 0.9339, n<sub>20</sub>D 1.5073, [α]<sub>20</sub>D 141°, and IV, d<sub>20</sub> 0.9378, n<sub>20</sub>D 1.5135, [α]<sub>20</sub>D 167.5°. Treatment of I with LiBH<sub>4</sub> and BF<sub>3</sub>·Et<sub>2</sub>O in Et<sub>2</sub>O and subsequent oxidation with Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in boiling H<sub>2</sub>SO<sub>4</sub> afforded V, m. 88-9° (Et<sub>2</sub>O-petroleum ether), [α]<sub>20</sub>D 40.5° (CHCl<sub>3</sub>), which yielded with SOCl<sub>2</sub> in pyridine VI, b<sub>0.01</sub> 135-40°. Hydrogenation of VI and subsequent treatment of the resulting saturated ketone with HSCH<sub>2</sub>CH<sub>2</sub>SH and BF<sub>3</sub>·Et<sub>2</sub>O in AcOH gave VII, b<sub>0.001</sub> 180°, which was refluxed 6 hrs. with Raney Ni in dioxane to yield eremophilane, b<sub>15</sub> 140°, [α]<sub>20</sub>D 36.4°. The ir, 1H N.M.R., and mass spectra were determined and discussed.

L16 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1969:58051 HCAPLUS

DOCUMENT NUMBER: 70:58051

TITLE: Total synthesis of (+)-nootkatone

AUTHOR(S): Odom, Homer C.; Pinder, Albert R.

CORPORATE SOURCE: Clemson Univ., Clemson, SC, USA

SOURCE: Chemical Communications (London) (1969), (1), 26-7

CODEN: CCOMA8; ISSN: 0009-241X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The Michael addition of di-Et malonate to acrylonitrile gave the dinitrile (EtO<sub>2</sub>C<sub>2</sub>)<sub>2</sub>C(CH<sub>2</sub>CH<sub>2</sub>CN), which was hydrolyzed, decarboxylated, and reesterified to MeO<sub>2</sub>CCH(CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Me)<sub>2</sub>. Dieckmann cyclization of the latter compt. gave di-Me 4-oxo-1,3-cyclohexane dicarboxylate, which was methylated to di-Me 3-methyl-4-oxo-1,3-cyclohexanedicarboxylate (I). I was hydrolyzed and decarboxylated to give cis-3-methyl-4-oxocyclohexanecarboxylic acid. This compound was converted to its dithio acetal with HSCH<sub>2</sub>CH<sub>2</sub>SH and treated with MeLi to give II (X = O). A Wittig reaction with methylenetriphenylphosphorane gave II (X = CH<sub>2</sub>), which was hydrolyzed with mercuric ion in MeOH to cis-4-isopropenyl-2-methylcyclohexanone (III). The annulation of III with trans-3-penten-2-one in the presence of NaH gave (±)-nootkatone, m. 45-6°, which was isolated by fractional distillation and column and preparative thin-layer chromatog., and which was identical in spectral and chromatographic properties with a sample of natural (-)-nootkatone.

L16 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1968:506902 HCAPLUS

DOCUMENT NUMBER: 69:106902

TITLE: The total synthesis of racemic nootkatone

AUTHOR(S): Pesaro, Mario; Bozzato, Giuliano; Schudel, Peter

CORPORATE SOURCE: Res. Co., Givaudan-Esrolko Ltd., Duebendorf/Zurich, Switz.

SOURCE: Chemical Communications (London) (1968), 19, 1152-4

CODEN: CCOMA8; ISSN: 0009-241X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 69:106902

GI For diagram(s), see printed CA Issue.

AB dl-Nootkatone (I) was prepared by treating

4-acetyl-1-ethoxycyclohexene with triphenylmethyl-phosphonium iodide in tetrahydrofuran in the presence of BuLi, followed by mild acid hydrolysis. NaOMe catalyzed the condensation of the resulting II (R = H<sub>2</sub>), b<sub>20</sub> 102-3°, with HCO<sub>2</sub>Et to give II (R = CHO), b<sub>0.005</sub> 55-60°, which on treatment with MeI in Me<sub>2</sub>CO gave a mixture (A) of ketoaldehydes: II (R = α-Me, β-CHO) (III), b<sub>0.01</sub> 55-65°, and II (R = β-Me, α-CHO) (IV), b<sub>0.01</sub> 55-65°; and II (R = CHOMe). Condensation of III and IV with Me<sub>2</sub>CO in the presence of piperidine-HOAc and treatment of the product with MeOH-KOH gave V (R<sub>1</sub> = R<sub>2</sub> = H) (VI), m. 39-40°, and VII, b<sub>0.01</sub> 122-4°, resp., which were separated by crystallization Reductive methylation of VI

with

Li+Me<sub>2</sub>Cu- in anhydrous Et<sub>2</sub>O at 0° gave 85% 4-epinootkatone (VIII), b<sub>0.004</sub> 75-80°, which on dehydrogenation with 2,3-dichloro-5,6-dicyanobenzoquinone in PhMe gave dl-V (R<sub>1</sub> = H, R<sub>2</sub> = Me) (IX), b<sub>0.001</sub> 100-5°. Condensation of A with AcCH<sub>2</sub>CO<sub>2</sub>Me in the presence of piperidine-HOAc, followed by treatment with KOH and CH<sub>2</sub>N<sub>2</sub> gave V (R<sub>1</sub> = CO<sub>2</sub>Me, R<sub>2</sub> = H), m. 78-9°, which on methylation gave >80% of a crystalline keto ester (X), m. 94-5°, and traces of its epimer m. 132-3°. X on saponification and decarboxylation gave VIII. X on dehydrogenation, as VIII, gave V (R<sub>1</sub> = CO<sub>2</sub>Me, R<sub>2</sub> = Me), b<sub>0.005</sub> 135-40°, which on reduction with NaBH<sub>4</sub> in pyridine, saponification, and decarboxylation gave crystalline I, m. 45-6°.

The

uv, ir, and N.M.R. spectra of the intermediate products are given.

L16 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:516969 HCAPLUS

DOCUMENT NUMBER: 67:116969

TITLE: Total synthesis of racemic isonootkatone (α-vetivone)

AUTHOR(S): Marshall, James A.; Faubl, Hermann; Warne, Thomas M., Jr.

CORPORATE SOURCE: Northwestern Univ., Evanston, IL, USA

SOURCE: Chemical Communications (London) (1967), (15), 753-4  
CODEN: CCOMA8; ISSN: 0009-241X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 67:116969

GI For diagram(s), see printed CA Issue.

AB I is prepared and used to synthesize compds. of the general formula II and the II are used in the preparation of III(α-vetivone). Also prepared is IV. Thus, Me<sub>2</sub>C:C(CO<sub>2</sub>Et)<sub>2</sub> is treated with LiAlH<sub>4</sub> to give Me<sub>2</sub>C:C(CH<sub>2</sub>OH)<sub>2</sub>, b<sub>0.2</sub> 78°, which is treated with PBr<sub>3</sub> in ether-hexane-pyridine to give Me<sub>2</sub>C:C(CH<sub>2</sub>Br)<sub>2</sub>, and the dibromide is treated with NaCH(CO<sub>2</sub>Et)<sub>2</sub> to give Me<sub>2</sub>C:C[CH<sub>2</sub>CH(CO<sub>2</sub>Et)<sub>2</sub>]<sub>2</sub> (V). V is hydrolyzed and the acid is decarboxylated to give Me<sub>2</sub>C:C(CH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>H)<sub>2</sub> which is converted to the di-Me ester, b<sub>0.2-0.3</sub> 87-95°; and the diester is treated with NaH to give Me 4-isopropylidenecyclohexanone-2-carboxylate (VI), b<sub>0.03-0.04</sub> 67-75°. VI is treated with trans-pent-3-en-2-ene in the presence of NaOMe(MeOH), addnl. NaOMe is introduced, and the mixture is kept about 18 hrs. at room temperature to give

I; a

mixture of I, HOCH<sub>2</sub>CH<sub>2</sub>OH, p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H, and C<sub>6</sub>H<sub>6</sub> is refluxed to give II (R = CO<sub>2</sub>Me) (VII). VII is treated with LiAlH<sub>4</sub> in ether to give II (R = CH<sub>2</sub>OH); II (R = CH<sub>2</sub>O<sub>3</sub>SMe) is treated with Li in NH<sub>3</sub>-EtOH to give a mixture containing II (R = CH<sub>2</sub>OH) and II (R = Me), and the mixture is hydrolyzed to give III. II (R = CH<sub>2</sub>O<sub>3</sub>SMe) is treated with LiAlH<sub>4</sub> in ether to give IV. N.M.R. and uv data are given.

L16 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:443943 HCAPLUS  
DOCUMENT NUMBER: 67:43943  
TITLE: Structure of  $\alpha$ -vetivone (isonootkatone)  
AUTHOR(S): Marshall, James A.; Andersen, Niels H.  
CORPORATE SOURCE: Northwestern Univ., Evanston, IL, USA  
SOURCE: Tetrahedron Letters (1967), (17), 1611-15  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Separation of ketonic components of Haiti oil of vetiver with Girard reagent T and partition of Javanese vetivert acetate between C<sub>6</sub>H<sub>14</sub> and 1:1:5 C<sub>5</sub>H<sub>5</sub>N-H<sub>2</sub>O-MeOH gave vetivones separated from each other and various contaminants by preparative gas chromatog. on a 20% Carbowax 20-M on Chromosorb W at 205° to give  $\alpha$ -vetivone (I), C<sub>15</sub>H<sub>22</sub>O, (mass spectrum), m. 30-5°, n<sub>D</sub> 1.5384, [ $\alpha$ ]<sub>D</sub> 20D 248°, 202° (CHCl<sub>3</sub>, dioxane), [ $\alpha$ ]<sub>D</sub> 405 570° (dioxane). In addition to the expected signals for vinyl H, Me<sub>2</sub>C:, and Me-CH groupings at 5.78, 1.70, 0.92 (doublet) (J 6 Hz) ppm., resp., the N.M.R. spectrum showed a prominent 3-proton singlet at 0.91 ppm. but no peak suggestive of a Me substituent on the  $\beta$ -position of an  $\alpha,\beta$ -unsatd. ketone. I treated with Li in NH<sub>4</sub>OH-EtOH followed by oxidation with CrO<sub>3</sub> gave a dihydro- $\alpha$ -vetivone (II). II brominated and spontaneously dehydrobrominated gave the trienone (III), also prepared by treating I with chloranil or 2,3-dichloro-5,6-dicyano-1,4-benzoquinone, and identified as isodehydronootkatone by ir, N.M.R., and uv spectra. The absolute configuration of I was assigned from the published O.R.D. curve (Djerassi, et al., CA 51: 5110a) which shows a pos. Cotton effect. Substitution of the name isonootkatone for  $\alpha$ -vetivone is recommended. Uv and ir spectral data were given.

L16 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:432806 HCAPLUS  
DOCUMENT NUMBER: 67:32806  
TITLE: Structure of valerianol, a sesquiterpenic alcohol of eremophilane type from Valeriana oil  
AUTHOR(S): Jommi, Giancarlo; Krepsinsky, Jiri; Herout, Vlastimil; Sorm, Frantisek  
CORPORATE SOURCE: Czechoslov. Acad. Sci., Prague, Czech.  
SOURCE: Tetrahedron Letters (1967), (8), 677-81  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB From the essential oil of V. officinalis a new alc., valerianol (I), C<sub>15</sub>H<sub>26</sub>O, n<sub>D</sub> 1.5117, [ $\alpha$ ]<sub>D</sub> 20D 134° (CHCl<sub>3</sub>), b<sub>D</sub> 0.01 120°; 3,5-dinitrobenzoyl derivative, m. 148°, was isolated. I contained a double bond, OH, Me, and secondary Me groups. Dehydrogenation with S gave eudalene, suggesting the presence of I of eremophilane or selinane carbon skeletons. Treatment of I with OsO<sub>4</sub> and C<sub>5</sub>H<sub>5</sub>N in Et<sub>2</sub>O gave the triol (II), m. 149-50°, [ $\alpha$ ]<sub>D</sub> 20D 32.6° (CHCl<sub>3</sub>), containing >CMe<sub>2</sub>,  $\rightarrow$  CMe, >CHMe, and CH<sub>2</sub>OH groups, and excluding location of the double bond in the selinane skeleton. Dehydration of I with POCl<sub>3</sub> or SOCl<sub>2</sub> or pyrolysis of the dinitrobenzoate gave no conjugated diene and excluded the selinane skeleton. I hydrogenated over prerduced PtO<sub>2</sub> gave dihydrovalerianol (III), thus locating the double bond in positions 9,10 or 1,10 on the eremophilane skeleton. Dehydration of I gave a 3:1 mixture

of hydrocarbons (IV and V). IV, C<sub>15</sub>H<sub>24</sub>, d<sub>20</sub> 0.9339, n<sub>20D</sub> 1.5073, [α]<sub>20D</sub> 141°, V, d<sub>20</sub> 0.9378, n<sub>20D</sub> 1.5135, [α]<sub>20D</sub> 167.5°. I treated with B<sub>2</sub>H<sub>6</sub> and oxidized according to Brown and Garg (CA 56: 9983e) gave an oxo alc. (VI), m. 88-9°, [α]<sub>20D</sub> 40.5° (CHCl<sub>3</sub>), not isomerized on refluxing in 5% KOH-MeOH and dehydrated to 2 unsatd. ketones (VII and VIII). VIII hydrogenated over Pd-C in MeOH gave a saturated ketone, converted by treatment with HSCH<sub>2</sub>CH<sub>2</sub>SH and BF<sub>3</sub>.Et<sub>2</sub>O in AcOH to give the ethylene thio ketal (IX), m/e 298, base peak m/e 131 and not m/e 173, showing the double bond to be located at position 1,10. The naturally occurring valencene (MacCleod, CA 64: 12730b) and the hydrocarbon from I are identical and provide unequivocal proof of the absolute stereochemistry of I, another member of the family (nootkatone, valencene, and nootkatene) with unusual eremophilane skeleton.

L16 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1966:67999 HCAPLUS

DOCUMENT NUMBER: 64:67999

ORIGINAL REFERENCE NO.: 64:12730b-f

TITLE: Constitution of nootkatone, nootkatene, and valencene

AUTHOR(S): MacCleod, William D., Jr.

CORPORATE SOURCE: U.S. Dept. Agr., Pasadena, CA

SOURCE: Tetrahedron Letters (1965), (52), 4779-83

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 62, 5808h. The mildly pungent sesquiterpene ketone, nootkatone (I), valued for its contribution to the distinctive flavor of grapefruit, Citrus paradisi has spectral bands at  $\nu$  1672, 1620, 1415, 895 cm.<sup>-1</sup>,  $\lambda$  237 m $\mu$  ( $\epsilon$  17,000). The Me doublet in the N.M.R. spectrum  $\delta$  0.9 d (6), 1.1 s, 1.7 t (.apprx.1), 2.1, 4.7 a (.apprx.1), 5.6 s excludes structures lacking the -CHMe- part structure. Oxidation of I with chloranil in hot AcOH gave dehydronootkatone,  $\lambda$  281 m $\mu$  ( $\epsilon$  23,000), N.M.R. spectrum similar to that of I with added peaks centered at  $\delta$  6.1 and 6.2. Isomerization in alc. KOH gave isodehydronootkatone,  $\lambda$  347 m $\mu$  ( $\epsilon$  24,000),  $\nu$  1415 cm.<sup>-1</sup>, N.M.R. AB doublets at  $\delta$  5.8, 6.4 (10), 1.8. Tetrahydronootkatone (II) brominated in AcOH gave the 3-bromo derivative (III), m. 80-1°,  $\delta$  5.3 (J = 11 cycles/sec.) requiring axial orientation of the H-3 and H-4 protons and consequent equatorial orientation of C-4 Me and C-3 Br. III dehydrobrominated in refluxing collidine gave a dihydronootkatone (IV),  $\lambda$  238 m $\mu$  ( $\epsilon$  13,000), N.M.R. showing signals  $\delta$  5.6 (.apprx.2), 1.9 (.apprx.2), (1.0, indicating the position of the vinyl Me  $\beta$  to the CO group. The tertiary Me group present in all compds. at C-5 serves to block tautomerism of the dienone (V) to a phenol. IV was isomeric with a hydrogenation product of I,  $\lambda$  238 m $\mu$  ( $\epsilon$  17,000). Both isomers could be reduced to II or oxidized with dichlorodicyanoquinone to V,  $\lambda$  244 m $\mu$  ( $\epsilon$  17,000). The O.R.D. curves of I and II showed pos. Cotton effects similar to those of cholest-4-en-3-one and cholestanone, resp. The amplitude of the curve of II in MeOH diminished markedly suggesting the presence of an equatorial Me group at C-4. Ketone (VI, R = O) submitted to modified Wolff-Kishner reduction gave the corresponding saturated hydrocarbon VI (R = H<sub>2</sub>) with ir spectrum and opposite optical rotation of the same magnitude as that of (+)-nootkatone, [α]<sub>D22°</sub>, thus confirming the constitution of I. I oxidized with alkaline H<sub>2</sub>O<sub>2</sub> and the nootkatone oxide, m. 47-8°, treated with N<sub>2</sub>H<sub>4</sub>-alc.-AcOH gave the hydroxydiene, readily dehydrated by treatment with POCl<sub>3</sub> in hot C<sub>5</sub>H<sub>5</sub>N to a triene,

identical to natural nootkatene (VII). Wolff-Kishner reduction of I yielded valencene (VIII), reconverted to I with tert-Bu<sub>2</sub>CrO<sub>4</sub>. I, VII, and VIII are a new and biogenetically interesting series of sesquiterpenes which are exceptions to the isoprene rule, but not to  $\beta$ -orientation of the isopropylene group.

L16 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1966:52221 HCAPLUS

DOCUMENT NUMBER: 64:52221

ORIGINAL REFERENCE NO.: 64:9771g-h, 9772a-g

TITLE: Constituents of atractylodes. X. Correlation of hinesol and  $\beta$ -vetivone

AUTHOR(S): Yoshioka, Ichiro; Kimura, Takeatsu

CORPORATE SOURCE: Univ. Osaka, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1965), 13(12), 1430-4

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 61, 9533c. Hinesol (I) was proposed (CA 55, 23382i) the structure Ia which was modified to Ib by Chow, et al. (CA 58, 1497d). Oxidation of I with SeO<sub>2</sub> in boiling dioxane for 4 h. gave an oil which gave a pos. 2,4-dinitrophenylhydrazine-H<sub>2</sub>SO<sub>4</sub> test, exhibited absolute maximum at 233.5 m $\mu$  (log  $\epsilon$  3.99) in the uv spectrum, and OH, C:CHO, CH<sub>2</sub>C: in the ir spectrum. These data suggested structure II and hence formula Ib must be preferred over Ia. Oxidation of a solution of 0.7 g. I in 10 mL. pyridine with 1 g. CrO<sub>3</sub> in 10 mL. pyridine and chromatog. of the product on Al<sub>2</sub>O<sub>3</sub> gave 0.2 g. unreacted I and 0.38 g. 4-oxohinesol (III), m. 73.5°, [ $\alpha$ ]<sub>D</sub> -91.3° (c 3.56, CHCl<sub>3</sub>). Structure III was well supported by its uv, ir, and N.M.R. spectra. It was expected that III on dehydration would give a compound of vetivone type. III (216 mg.) was heated with 440 mg. KHSO<sub>4</sub> at 190-210° for 2 h. and the product distilled to give an oil b<sub>5</sub> 160-80° which showed 7 peaks in its gas chromatogram one of which was due to  $\beta$ -vetivone known to have structure IV. Dehydration of 103 mg. III with 0.3 mL. HCO<sub>2</sub>H at 120-30° for 1 h. gave a yellow oil, b<sub>2</sub> 110-20°, whose gas chromatogram showed 3 peaks one of which was due to IV. The oil was a mixture and its spectra indicated a mixture of structures expressed as V. The oils in the above 2 reactions could not be purified further. Refluxing 117 mg. III with 2.5 mL. Ac<sub>2</sub>O for 4 h. gave 100 mg. 4-oxohinesol acetate (VI), b<sub>3</sub> 150-65°, semicarbazone, m. 178°. Treatment of 101 mg. VI in 2 mL. ether with 0.3 BF<sub>3</sub>-etherate at room temperature for 1 h. gave an oil (VII), b<sub>2</sub> 135-40° whose gas chromatogram showed one main peak corresponding to IV and 2 minor peaks. VII was therefore converted into semicarbazone which on recrystn. gave 4-oxo- $\Delta^9$ (11)-hinesene semicarbazone (VIII), m. 222°, [ $\alpha$ ]<sub>D</sub> 62.2° (c 4.28, HOAc). Hydrolysis of 260 mg. VIII with 260 mg. phthalic anhydride and 30 mL. H<sub>2</sub>O under reflux for 9 h. gave 66.5 mg. 4-oxo- $\Delta^9$ (11)-hinesene (X), b<sub>3</sub> 140-3°, [ $\alpha$ ]<sub>D</sub> 38.03° (c 0.66, EtOH); 2,4-dinitrophenylhydrazone (XI), m. 188-91°. For comparison, IV was obtained from vetiver oil and converted into its 2,4-dinitrophenylhydrazone (XII), m. 188-91°. The ir spectra of X and XI were exactly superimposable on those of IV and XII. However the m.p. of a mixture of XI and XII was depressed (158-62°). The ORD (O.R.D.) curves of X and IV were sym. indicating that X is the enantiomer of IV. This conclusion was further supported by the fact that the rotation of VIII was 62.2° while that of IV semicarbazone is -71.1°. Since the relative configuration of H atoms at C-1 and C-7 of IV and  $\alpha$ -vetivone (XIII) was established by Naves and

Perottet (CA 35, 47555) as cis and the absolute configuration of C-6 Me as S by Sorm, it was concluded that hinesol must be 1S, 6S, 7S as in XIV or 1R, 6S, 7R as in XV. Also  $\alpha$ -vetivone and  $\beta$ -vetivone must be represented as XIII and IV, resp.

L16 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1963:409156 HCAPLUS

DOCUMENT NUMBER: 59:9156

ORIGINAL REFERENCE NO.: 59:1691a-g

TITLE: The chemistry of the natural order Cupressales. XLVI.  
The structure of nootkatone

AUTHOR(S): Erdtman, Holger; Hirose, Yoshiyuki

CORPORATE SOURCE: Kungl. Tek. Hogskolan, Stockholm

SOURCE: Acta Chemica Scandinavica (1962), 16, 1311-14

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB A new sesquiterpene ketone, nootkatone, has been isolated from the neutral fraction of the acetone extract of *Chamaecyparis nootkatensis* by two methods. The neutral fraction from 28 kg. heartwood (370 g.) was distilled through a fractionating column and the fractions b. 156-8°/5 mm. were redistd. through a spinning band column. Series of fractions boiling between 154 and 155° were obtained, the optical rotation of which varied from  $[\alpha]_D^{25} 91^\circ$  to  $148^\circ$ . They were dissolved in 6 times their volume of EtOH and treated with NaOAc and semicarbazide-HCl to give 25 g. crystals, which gave 15 g. pure nootkatone semicarbazone. A mixture of the latter with 15 g. Bz2O and 45 ml. H2O was steam distilled and the distillate extracted with ether to give 5 g. nootkatone (I) as an oil, m. 36-7°,  $[\alpha]_D^{25} 195.5^\circ$  (c 1.5, CHCl3),  $\lambda$  238 m $\mu$  ( $\epsilon$  15,000),  $\nu$  1680 cm.<sup>-1</sup>, and the formula C15H22O. In the second method, the fraction b5 155-180° (105 g.) and 16 g. Girard P reagent were dissolved in 300 ml. EtOH containing 30 g. HOAc and refluxed 40 min. After cooling it was poured into 2 l. H2O containing 27 g. Na2CO3 and the mixture extracted with ether to give 10 g. of a brownish oil which crystallized from

petr.

ether to give pure I; I semicarbazone m. 195-7°; 2,4-dinitrophenylhydrazone m. 157.5°. The ultraviolet and infrared spectra of I clearly showed that I is an  $\alpha,\beta$ -unsatd. ketone and is thought to have the structure given. The ozonization of 118 mg. I in 20 ml. CH2Cl2 gave only HCHO isolated as its dimedon derivative but no acetone was isolated. I (51.9 mg.) in EtOH in the presence of Pd-C was hydrogenated to give tetrahydronootkatone (II) as a viscous oil; its semicarbazone m. 210-11° (decompn.),  $[\alpha]_D^{25} 66.5^\circ$  (c 0.09, CHCl3). In the presence of Adams catalyst 120 mg. I was hydrogenated to give a product, which after chromatography gave 30% oil and 70% crystals. The latter, tetrahydronootkatol (III), m. 76.5-77°,  $[\alpha]_D^{25} 13.9^\circ$  (c 2.2, CHCl3). Oxidation of 320 mg. III in 5 ml. pyridine with 400 mg. CrO3 in 5 ml. pyridine overnight gave a liquid, b6 152°, nD 1.4886,  $[\alpha]_D^{25} 54.1^\circ$  (c 2.4, CHCl3), whose semicarbazone was identical with that of II. A sample of II prepared by oxidation of III was purified by ozonizing the unsatd. impurities and had  $[\alpha]_D^{25} 19.2^\circ$ . Reduction of 300 mg. I in 5 ml. MeOH with 300 mg. KBH4 overnight gave 300 mg. of a viscous, uncrystallizable oil. The latter was heated with 300 mg. Se 12 hrs. to give eudalene isolated as its picrate. To locate the CO group, 1.3 g. II in 5 ml. ether was treated with MeMgBr prepared from 0.2 g. Mg and 1.5 g. MeI in 5 ml. ether. After keeping overnight, it gave 0.9 g. of a pale yellow alc.,  $\nu$  3620 cm.<sup>-1</sup>, with no CO band. On heating this alc. with Se at

330° 30 hrs. it gave 0.4 g. liquid; picrate m. 104-6°; trinitrobenzene adduct m. 121-2°. These were identical with the corresponding derivs. of 1,3-dimethyl-7-isopropyl-naphthalene. The proton magnetic resonance spectrum of I in CCl<sub>4</sub> showed a signal at 62 cycles/sec. due to a single proton on a double bond. The low frequency is due to the proton being next to a CO group. A signal at 103 cycles/sec. was due to 2 H atoms on terminal methylene group of isopropenyl group. Three sharp lines at 250, 223, and 207 cycles/sec. corresponded to three Me groups of which the last is due to a Me group in the system of the type COCH: CMe. All these facts favor structure I. The configuration at C7 is not known with certainty. It is present as  $\beta$  in eudesmol and the phys. properties of I suggest it to be similarly oriented in I. If it is correct, the Me group at C4 and the OH at C2 in III should be  $\beta$ -oriented, hydrogenation occurring at the least hindered side.

L16 ANSWER 36 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1939:41328 HCAPLUS

DOCUMENT NUMBER: 33:41328

ORIGINAL REFERENCE NO.: 33:5832b-h

TITLE: Volatile plant constituents. X. The vetivones, odorous constituents of the essential oils of vetiver

AUTHOR(S): St. Pfau, Alexander; Plattner, Pl. A.

SOURCE: Helvetica Chimica Acta (1939), 22, 640-54

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB C. A. 33, 4960.3. The use of phenylhydrazinesulfonic acid or of acetylhydrazinopyridinium chloride (cf. Girard and Sandulesco C. A. 31, 1006.4) to isolate the ketones from essential oil of vetiver did not prove satisfactory. A ketonic fraction (254 g.) of oil of vetiver, b<sub>4</sub> 152-60° and containing 81.5% C<sub>15</sub>H<sub>22</sub>O according to oxime anal., gave 255.3 g. of crude semicarbazone (97.6% yield). Fractional crystallization of

the

crude semicarbazone yields the semicarbazone of  $\beta$ -vetivone, C<sub>16</sub>H<sub>25</sub>ON<sub>3</sub> (I), m. 228-9°, [ $\alpha$ ]<sub>D</sub><sup>20</sup> -71°, soluble in AcOH without color and a light d-rotatory powder, soluble in AcOH with yellow color. Fractional crystalline of this powder from EtOH yields the semicarbazone of  $\alpha$ -vetivone, C<sub>16</sub>H<sub>25</sub>ON<sub>3</sub> (II), m. 210-12° (decomposition), [ $\alpha$ ]<sub>D</sub><sup>20</sup> 316°, and a mixture of semicarbazones, [ $\alpha$ ]<sub>D</sub><sup>20</sup> 120 to +160°. The ketone fraction from oil of vetiver varies from about 20 to 90% and the yield of  $\beta$ -vetivone from 2 to 49%. Refluxing 110 g. I, 230 g. phthalic anhydride and 800 mL. water for 12 h., neutralizing and extracting with Et<sub>2</sub>O gave 65 g. (82% theory)  $\beta$ -vetivone oil, b<sub>10</sub> 175°, and II gave similarly  $\alpha$ -vetivone. Crystallization of  $\beta$ -vetivone oil from petr. ether gave a poor yield of  $\beta$ -vetivone (III), m. 44-4.5°, [ $\alpha$ ]<sub>D</sub><sup>20</sup> -24.1°. III forms no bisulfite compound III (20 g.), 20 g. KOH, 0.5 g. CuSO<sub>4</sub> and 20 mL. water heated by the Kijner-Wolff method gave 6.5 g. C<sub>15</sub>H<sub>24</sub>, b<sub>2.5</sub> 110-2°, d<sub>20</sub> 0.9244, n<sub>D</sub><sup>20</sup> 1.5116. When 50 g. III was treated repeatedly with Al and iso-PrOH it gave 5.5 g. of C<sub>15</sub>H<sub>22</sub>, b<sub>3.6</sub> 110°, d<sub>20</sub> 0.9277, n<sub>D</sub><sup>20</sup> 1.5277. Reduction of 65 g. III with alc. and Na gave a distillate which partly solidified and these crystals, recrystd. from acetone and petr. ether and sublimed under reduced pressure, gave  $\beta$ -dihydrovetivol, m. 103.5°. Catalytic hydrogenation of III gave a  $\beta$ -dihydrovetivol (IV), m. 107°; dinitrobenzoate, m. 121° and remelts at 129.5-30°. Probably catalytic hydrogenation gave a single stereoisomer and reduction with Na a mixture. Some  $\beta$ -dihydrovetivone (dibenzylidene derivative, m. 130.5-1.5°) was also formed as a byproduct of catalytic hydrogenation. Catalytic

hydrogenation of IV gave  $\beta$ -tetrahydrovetivol (V), m. 76-6.5°; dinitrobenzoate, m. 144-4.5°. V is also obtained by direct hydrogenation of III. Oxidation of V with Cr<sub>2</sub>O<sub>3</sub> and AcOH gave  $\beta$ -tetrahydrovetivone m. 37.5-8° (dibenzylidene derivative m. 101.5-2°). Reduction of 10.4 g. of mixed ketones obtained from the d-rotatory semicarbazones with Na and alc. gave a mixture of dihydroisovetivols, C<sub>15</sub>H<sub>26</sub>O, b<sub>4</sub> 153°, d<sub>20</sub> 0.9858, n<sub>D20</sub> 1.5159,  $\alpha_D$  24.40°. The odor of the oil of vetiver is due principally to the ketonic sesquiterpenes, C<sub>16</sub>H<sub>22</sub>O, (bicyclic and  $\alpha$ -ethylenic) of which only  $\alpha$ -vetivone and  $\beta$ -vetivone have so far been isolated. Their derivs. so far prepared have little if any odor.

L16 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1939:38241 HCAPLUS  
DOCUMENT NUMBER: 33:38241  
ORIGINAL REFERENCE NO.: 33:5384e-h  
TITLE: Ketones of oil of vetiver  
AUTHOR(S): Sabetay, Sebastien; Trabaud, Lucien  
SOURCE: Bull. soc. chim. (1939), 6, 740-3  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

AB The structure of the principal constituents of oil of vetiver (I) is unknown. I contains 60% of vetiverols (II), C<sub>15</sub>H<sub>24</sub>O. The corresponding aldehydes are unknown and the presence of the ketones is disputed. By application of the methods of Girard and Sandulesco (C. A. 31, 1006.4) ketone fractions have been isolated from authentic Bourbon vetiver. Treatment of 500 g. I in 1.5 l. alc. and 75 g. AcOH with 75 g. of Girard reagent P gave 11.6% of crude ketone, n<sub>D20</sub> 1.5319, d<sub>415</sub> 1.0038,  $\alpha$  71.20°, containing 84.8% of vetiverone (III). Distillation in vacuo gave a principal fraction, b<sub>14</sub> 138-48°, of which 20 g. was converted into 21 g. of crude semicarbazone from which was regenerated 5 g. of the sesquiterpenic ketone III, C<sub>15</sub>H<sub>22</sub>O, b<sub>12</sub> 142-50°, n<sub>D20</sub> 1.5252, d<sub>415</sub> 1.002,  $\alpha$  74° (10 cm.), giving brownish red and violet colors with SbCl<sub>3</sub> and Br in AcOH; semicarbazone, m. 210°. Similarly a Java vetiver gave a sample of II, b<sub>20</sub> 150-5°, n<sub>D20</sub> 1.5355, d<sub>415</sub> 1.001,  $\alpha$  80.40° (10 cm.); semicarbazone, m. 210°. Oxidation of 45 g. II (free from III) with 60 g. K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and 50 g. H<sub>2</sub>SO<sub>4</sub> in 300 cc. H<sub>2</sub>O yielded 12 g. of crude vetiveral, b<sub>10</sub> 138-45°, n<sub>D20</sub> 1.5132, d<sub>415</sub> 1.003,  $\alpha$  40.55° (10 cm.), containing 64.1% of vetiveral, C<sub>15</sub>H<sub>22</sub>O (as determined by oximation).

=> => d stat que l24

L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?  
L2 SEL PLU=ON L1 1- CHEM : 100 TERMS  
L3 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L2  
L4 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L3 OR NOOTKATON?  
L5 7087 SEA FILE=HCAPLUS ABB=ON PLU=ON (TICKS/CV OR ACARI/CV) OR  
TICK OR ACARI OR ANTITICK? OR ANTIACARI?  
L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND L5  
L7 194193 SEA FILE=HCAPLUS ABB=ON PLU=ON PESTICIDES/CV OR ACARICIDES/CV  
OR INSECTICIDES/CV OR RODENTICIDES/CV REPELLENTS/CV OR  
PESTICIDE OR INSECTICIDE OR RODENTICIDE OR REPELLENT  
L8 16 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND L7) NOT L6  
L9 4916981 SEA FILE=HCAPLUS ABB=ON PLU=ON MATERIAL OR SOIL OR POLYMER?  
OR DIATOMACEO? OR DIATOMITE OR SAND OR CELLULOSE  
L10 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L4(L)L9  
L11 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT (L6 OR L8)  
L15 42 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4(L)(TREAT? OR APPLY OR

APPLIED)) NOT (L6 OR L8)  
 L16 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L11  
 L23 26 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND (MULCH OR GRASS OR  
 ROOT OR ALUMIN? OR SILICA OR CLAY OR SOLID(W)SUBSTANC?)) NOT  
 (L6 OR L8 OR L11 OR L16)  
 L24 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND PD=<AUGUST 17, 2001

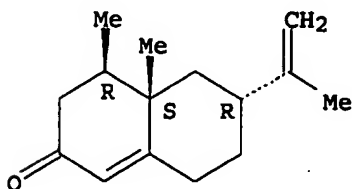
=>

=>

=> d ibib abs hitstr l24 1-16

L24 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2000:467347 HCAPLUS  
 DOCUMENT NUMBER: 133:149649  
 TITLE: Characteristic flavor compound in peel oil of lime  
 AUTHOR(S): Yang, Ronghua  
 CORPORATE SOURCE: Department of Food Science + Engineering, Hangzhou  
 Commercial College, Hangzhou, 310035, Peop. Rep. China  
 SOURCE: Shipin Yu Fajiao Gongye (2000), 26(3), 31-34  
 CODEN: SPYYDO; ISSN: 0253-990X  
 PUBLISHER: Shipin Yu Fajiao Gongye  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB The characteristic flavor compds. in peel oil of lime were studied by  
 solution extraction and silica gel column. Twenty-five compds.  
 including geraniol, neral, linalool and aliphatic aldehydes were selected as  
 the components contributed to the aroma of the peel oil.  
 IT 4674-50-4, Nootkatone  
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);  
 BIOL (Biological study); OCCU (Occurrence)  
 (characteristic flavor compound in peel oil of lime)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-  
 methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1993:58289 HCAPLUS  
 DOCUMENT NUMBER: 118:58289  
 TITLE: Characterization of grapefruit oil and juice by HPLC  
 AUTHOR(S): Schulz, Hartwig; Albroscheit, Gerd; Nowak, Dieter  
 CORPORATE SOURCE: Dragoco, Gerberding und Co., Holzminden, W-3450,  
 Germany  
 SOURCE: Zeitschrift fuer Lebensmittel-Untersuchung und  
 -Forschung (1992), 195(3), 254-8  
 CODEN: ZLUFAR; ISSN: 0044-3026  
 DOCUMENT TYPE: Journal

LANGUAGE: German

AB A rapid HPLC method for the determination of the flavor compound neotkatone (I) in

grapefruit oils and juices is described; the method also permits the detection of relevant coumarins and furocoumarins important for product quality evaluation. The oil is dissolved in hexane, cleaned-up on Bakerbond silica gel columns, eluting with MeOH for subsequent anal.; juices are extracted with EtOAc and the exts. are analyzed directly following solvent removal. Coumarin and furocoumarin detections require alc.-KOH refluxing, Et2O extraction, and preparative liquid chromatog.

isolation

before HPLC characterization. Nootkatone, coumarin and furocoumarin were chromatographed on Hypersil ODS columns with H2O-MeOH gradient elution and a diode array detection system. Nootkatone was detected at 240 nm, and coumarin and furocoumarin at 310 nm. The determination limit was 0.05% for nootkatone, with linearity for 0.1-1 mg/mL. Seven coumarins and furocoumarins were identified by NMR, mass spectroscopy, and combined chromatog.-MS techniques; relevant MS data are given.

IT 4674-50-4, Nootkatone

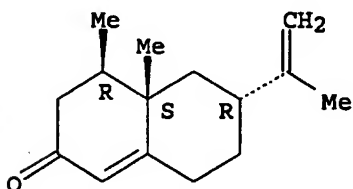
RL: ANT (Analyte); ANST (Analytical study)

(determination of, in grapefruit juice and oil, by HPLC)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:648544 HCAPLUS

DOCUMENT NUMBER: 117:248544

TITLE: Chemical constituents of volatile oil of Vladimiria soulier (Franch.) Ling

AUTHOR(S): Li, ZhaoLin; Xue, Dunyuan; Wang, Mingkui; Chen, Yaozu

CORPORATE SOURCE: Instrum. Anal. Res. Cent., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China

SOURCE: Lanzhou Daxue Xuebao, Ziran Kexueban (1991), 27(4), 94-7

CODEN: LCTHAF; ISSN: 0455-2059

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The volatile oil of the root of Vladimiria soulier (Franch.)

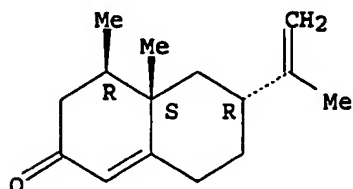
Ling was obtained by simultaneous distillation-extracting device from its dry root. The oil yield is 0.8%. The phys. and chemical constns. were determined and its chemical constituents have been analyzed by gas

chromatog./mass

spectrometry. Twenty-six components, constituting 75.41% of the oil, were identified by GC/MS. A colorless crystal was obtained by column chromatog. following recrystn., which was confirmed as dehydrocostus lactone. Thus, the major constituents of volatile oil of V. soulier is

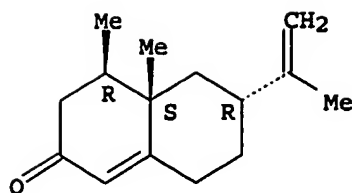
dehydrocostus lactone.  
 IT 4674-50-4, Nootkatone  
 RL: BIOL (Biological study)  
 (from Vladimiria soulier root volatile oil)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



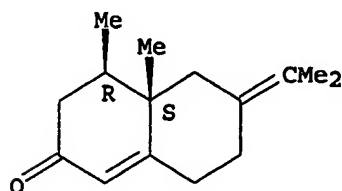
L24 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1992:547205 HCAPLUS  
 DOCUMENT NUMBER: 117:147205  
 TITLE: Biosynthesis of the constituents of vetiver oil II. Nootkatane and eudesmane compounds  
 AUTHOR(S): Akhila, Anand; Thakur, Raghunath S.  
 CORPORATE SOURCE: Cent. Inst. Med. Aromatic Plants, Lucknow, 226 016, India  
 SOURCE: Proc. - Int. Congr. Essent. Oils, Fragrances Flavours, 11th (1989), Volume 5, 143-50. Editor(s): Bhattacharyya, S. C.; Sen, N.; Sethi, K. L. Oxford & IBH: New Delhi, India. CODEN: 570QAS  
 DOCUMENT TYPE: Conference  
 LANGUAGE: English  
 AB [3RS;2-14C]MVA was incorporated into bicyclic sesquiterpenes of Vetiveria zizanioides in 4 + 10-3 to 6 + 10-3% yield. The roots of V. zizanioides which were fed with [2-14C; 4R-3H1]MVA and the isotope ratios in the compds. of nootkatane group such as isovalencenol, . alpha.-vetivone, isovalencenic acid, nootkatene, valencene, nootkatone, 7-epi-nootkatone, beta-vetivene, gamma-vetivene, bicyclovetivenol and valerianol suggest that a proton loss was followed by a 1,2-Me shift and a 1,2-hydrogen shift. A simple elimination reaction of a proton (electrophile) and an enzyme (nucleophile) takes place during the formation of iso-Pr or di-Me allyl grouping in the compds. of this group. On the other hand, 2 1,2-hydrogen shifts are observed, during the formation of levojunenol and a proton loss is followed by a 1,2-hydrogen shift in vetiselinene, isovetiselinenol, vetiselinenol, and delta-selinene.  
 IT 4674-50-4, Nootkatone 15764-04-2, alpha -Vetivone 34181-41-4  
 RL: PROC (Process)  
 (biosynthesis of, in Vetiveria zizanioides, from mevalonate, oil composition in relation to)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



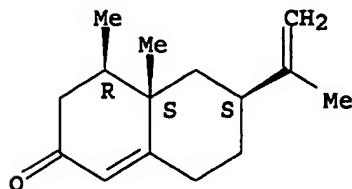
RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 34181-41-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, [4R-(4α,4aa,6α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1992:262270 HCAPLUS  
 DOCUMENT NUMBER: 116:262270  
 TITLE: Analysis of vetiver essential oil by supercritical fluid extraction and on-line capillary gas chromatography  
 AUTHOR(S): Blatt, Celso R.; Ciola, Remolo  
 CORPORATE SOURCE: Instr. Cient. CG LTDA, Sao Paulo, 04603, Brazil  
 SOURCE: Journal of High Resolution Chromatography (1991), 14(11), 775-7  
 CODEN: JHRCE7; ISSN: 0935-6304  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Vetiver oil was obtained by both supercrit. fluid and steam distillation extraction of the plant roots. Capillary gas chromatog. was performed on a silica column coated with poly(dione siloxane) or CG-FN-193 (siloxane) with flame ionization detection. Extraction at lower pressures resulted in a high recovery of sesquiterpene hydrocarbons and low recovery

of oxygenated compds. At higher pressures, the reverse was the case. The supercrit. fluid extraction method was more efficient than the steam distillation method.

IT 15764-04-2,  $\alpha$  -Vetivone

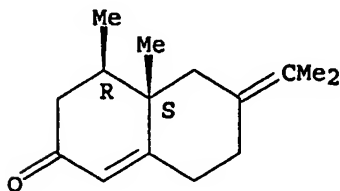
RL: BIOL (Biological study)

(of vetiver oil, supercrit. fluid extraction and capillary gas chromatog. in study of)

RN 15764-04-2 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:628369 HCAPLUS

DOCUMENT NUMBER: 115:228369

TITLE: Chemical composition of volatile oil of *Patrinia heterophylla* Bge

AUTHOR(S): Li, Zhaolin; Zhu, Jialiang; Chen, Ning; Chen, Yaozu

CORPORATE SOURCE: Anal. Test. Cent., Lanzhou Univ., Lanzhou, 730000, Peop. Rep. China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1991), 12(2), 213-15

CODEN: KTHPDM; ISSN: 0251-0790

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB The volatile oil of *P. heterophylla* root was obtained by simultaneous steam distillation-solvent extraction The yield of the oil was 0.63%.

Its chemical composition was studied by capillary gas chromatog.-mass spectrometry. Over 50 components were separated, of which 30 compds. composing 56.32% of the oil were identified. The major component, isovaleric acid, was separated by distillation under reduced pressure and identified

by MS, IR and NMR.

IT 4674-50-4, Nootkatone

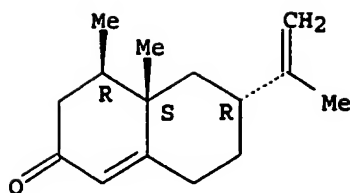
RL: BIOL (Biological study)

(from *Patrinia heterophylla* root volatile oil)

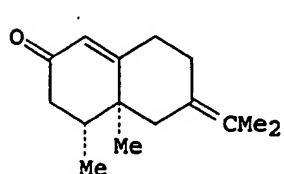
RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

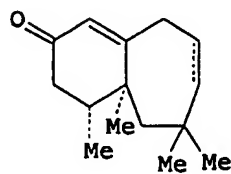
Absolute stereochemistry.



L24 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1990:164706 HCAPLUS  
 DOCUMENT NUMBER: 112:164706  
 TITLE: Resinoid and essential oil of Vetiver  
 AUTHOR(S): Retamar, J. A.; Elder, H. V.  
 CORPORATE SOURCE: Inst. Invest. Prod. Nat., Anal. Sint. Org., UNL, Santa Fe, 3000, Argent.  
 SOURCE: Essenze, Derivati Agrumari (1989), 59(1), 44-50  
 CODEN: EDAGAH; ISSN: 0014-0902  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

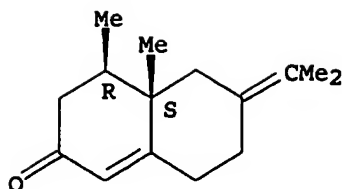


II, satd.

III, unsatd.

AB  $\alpha$ - (I) and  $\beta$ -vetivone, vetivenol, and vetivenyl vetivenate were the main constituents of the vetiver oil obtained by cohobation in a yield of 1.5%. Expansion and contraction of the I rings gave isomeric structures (II and III). Also, catalytic dehydration and dehydrogenation gave azulene structures. The oil had a hot and deep note with a great persistence. The resins (dried root exts.) had these characteristics in a higher degree.  
 IT 15764-04-2,  $\alpha$  -Vetivone  
 RL: BIOL (Biological study)  
 (of vetiver root oil and resin)  
 RN 15764-04-2 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:113410 HCAPLUS

DOCUMENT NUMBER: 110:113410

TITLE: Studies on the essential oils of pummelo. Part II. Changes in the volatile constituents of pummelo (Citrus grandis Osbeck forma Tosa-bun tan) during storage

AUTHOR(S): Sawamura, Masayoshi; Tsuji, Tetsuya; Kuwahara, Shigeru

CORPORATE SOURCE: Dep. Agric. Chem., Kochi Univ., Kochi, 783, Japan

SOURCE: Agricultural and Biological Chemistry (1989), 53(1), 243-6

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Changes in the volatile constituents of cold-pressed oil from pummelo during storage between Dec 10 and May 6 the following year were determined by silica gel column chromatog. Increases in terpene hydrocarbons and nootkatone were observed during storage, and the latter is considered as an indicator of best harvest time and postharvest ripening.

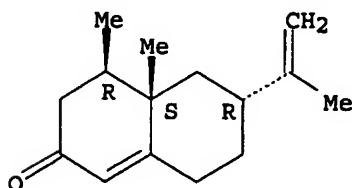
IT 4674-50-4, Nootkatone

RL: BIOL (Biological study)  
(of pummelo oil, fruit storage effect on)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:587488 HCAPLUS

DOCUMENT NUMBER: 109:187488

TITLE: Enhanced productivity of the essential oil in the artificial autopolyploid of vetiver (Vetiveria zizanioides L. Nash)

AUTHOR(S): Lavania, U. C.

CORPORATE SOURCE: Cent. Inst. Med. Aromatic Plants, Lucknow, 226016, India

SOURCE: Euphytica (1988), 38(3), 271-6

CODEN: EUPHAA; ISSN: 0014-2336

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Artificial autotetraploids were produced by colchicine treatment in the important essential oil bearing vetiver ( $2n = 20$ ). The raw tetraploids were stabilized by selection for pure types in segregating vegetative progeny. The tetraploids were vigorous with thicker and longer roots. The performance data recorded on the 17-mo-old crop of the tetraploid taken in conjunction with diploid parent and the best available check, exhibited distinct superiority of the tetraploid. In terms of economic yield the tetraploid has the potential of producing 62.5% and 39.2% more oil over the diploid parent and the check, resp. Although there was marginal improvement in root biomass, significant improvement was registered for percent oil content. The tetraploid produced 1.4% oil in freshly harvested roots compared to 0.98% and 1.15% in the control and check, resp. Thus, induced tetraploidy can be used in attaining rapid genetic improvement even for the characters associated with the secondary metabolism

IT 15764-04-2,  $\alpha$  -Vetivone

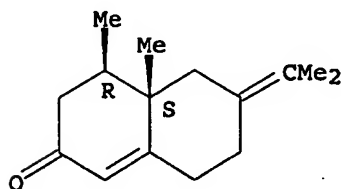
RL: BIOL (Biological study)

(in *Vetiveria zizanioides*, tetraploidy induction in relation to)

RN 15764-04-2 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethylidene)-, (4R,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:19239 HCAPLUS

DOCUMENT NUMBER: 108:19239

TITLE: Volatile compounds in peel oil of Shiroyanagi navel

AUTHOR(S): Sugisawa, Hiroshi; Yang, Rong Hua; Matsuo, Toshimasa; Tamura, Hirotoshi

CORPORATE SOURCE: Dep. Bioresour. Sci., Kagawa Univ., Miki, 761-07, Japan

SOURCE: Nippon Nogei Kagaku Kaishi (1987), 61(9), 1101-6

CODEN: NNKKAA; ISSN: 0002-1407

DOCUMENT TYPE: Journal

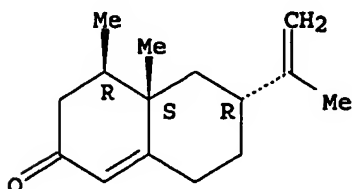
LANGUAGE: Japanese

AB The essential oil of Shiroyanagi navel (*Citrus sinensis* cv Shiroyanagi) was obtained from the peel by simultaneous distillation-extraction, and separated into

fractions of hydrocarbon and oxygenated compds. through a silica gel column. Both fractions were analyzed by combined capillary gas-chromatog.-mass spectrometry (GC/MS). Sixty-eight compds., including 9 hydrocarbons, 20 alcs., 20 aldehydes, 9 esters, 2 phenols, 4 ethers, and 4 ketones, were identified by GC/MS and Kovats Indexes. As the oxygenated fraction had the characteristic aroma of the oil, this fraction was further separated into 4 fractions, and then examined by GC/MS and GC-sniffing. The compositional characteristic of this oil was a large amount of terpene

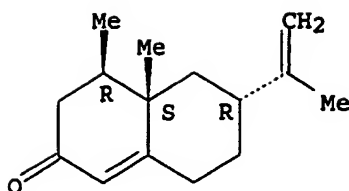
aldehyde compared with peel oils of other sweet oranges in Japan.  
 IT 4674-50-4, Nootkatone  
 RL: BIOL (Biological study)  
 (in peel oil of Citrus sinensis)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1987:514417 HCAPLUS  
 DOCUMENT NUMBER: 107:114417  
 TITLE: Terpene reduction in cold-pressed orange oil by frontal analysis-displacement adsorption chromatography  
 AUTHOR(S): Ferrer, O. J.; Matthews, R. F.  
 CORPORATE SOURCE: Food Sci. Hum. Nutr. Dep., Univ. Florida, Gainesville, FL, 32611, USA  
 SOURCE: Journal of Food Science (1987), 52(3), 801-5  
 CODEN: JFDSAZ; ISSN: 0022-1147  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Five adsorbents were studied for their ability to remove terpenes from cold-pressed Valencia orange oil by frontal-anal. displacement adsorption chromatog. Only the potable solvent 95% aqueous EtOH was used in the process; columns were dry-packed to eliminate the use of hexane. The most successful columns were silica gel and Florisil. Adsorptive capacities of 4.4 and 2.0 g oil/g adsorbent were achieved for silica gel and Florisil, resp. Compns. of the oil fractions were determined by gas chromatog. and peaks identified by mass spectrometry. Silica gel provided products with the lowest terpene level and the highest oxygenated compound content. The terpene content of the product considered best was reduced to one-fifth and one-seventh of the original level for Florisil and silica gel, resp., and had higher oxygenated compound levels than either 10-fold or 25-fold orange oil concs.  
 IT 4674-50-4, Nootkatone  
 RL: BIOL (Biological study)  
 (of orange oil, terpene hydrocarbons separation from, by adsorption column chromatog.)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1986:147331 HCAPLUS  
 DOCUMENT NUMBER: 104:147331  
 TITLE: Analysis of Cuban grapefruit peel oil  
 AUTHOR(S): Correria, M.; Tapanes, R.; Pino, J.  
 CORPORATE SOURCE: Natl. Cent. Sci. Res., Havana, Cuba  
 SOURCE: Acta Alimentaria (1985), 14(4), 303-8  
 CODEN: ACALDI; ISSN: 0139-3006  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Cold-pressed grapefruit peel oil was fractionated by silica gel column chromatog. with hexane and then MeOH, and the hydrocarbon fraction was distilled to sep. mono- and sesquiterpenes. The oxygenated compds. were fractionated by known methods, and all fractions were analyzed by gas chromatog. The oil contained 89.4% terpenes and 9.4% oxygenated compds. Of the 40 peaks separated, 28 compds. were identified, including 12 hydrocarbons, 8 aldehydes, and 8 alcs. The major compds. of each fraction were: monoterpenes limonene [138-86-3], sesquiterpenes caryophyllene [87-44-5] and  $\alpha$ -ylangene [14912-44-8], aldehydes decanal [112-31-2] and octanal [124-13-0], and alcs. linalool [78-70-6] and  $\alpha$ -terpineol [98-55-5]. Phys. and chemical characteristics agreed with those for the Florida oil.

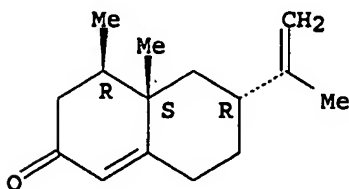
IT 4674-50-4

RL: BIOL (Biological study)  
 (of grapefruit peel oil)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

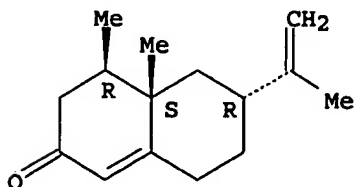
Absolute stereochemistry.



L24 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1984:119412 HCAPLUS  
 DOCUMENT NUMBER: 100:119412  
 TITLE: Quantitation of individual and total aldehydes in citrus cold-pressed oils by fused silica capillary gas chromatography  
 AUTHOR(S): Wilson, Charles W., III; Shaw, Philip E.  
 CORPORATE SOURCE: U. S. Citrus Subtrop. Prod. Lab., Winter Haven, FL,

33883, USA  
 SOURCE: Journal of Agricultural and Food Chemistry (1984), 32(3), 399-401  
 CODEN: JAFCAU; ISSN: 0021-8561  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Total aldehydes in cold-pressed oils from California and Florida citrus cultivars were quantified by fused silica capillary gas chromatog. using a nonpolar bonded-phase fused silica column (DB-5, 30m + 0.32 mm i.d., 1.0 µm film thickness; with H2 as the carrier gas). Total aldehydes by gas chromatog. were from 93 to 100% of the USP total aldehyde value and were within the limits of precision for the USP method. The major aldehydes quantified in oils were octanal [124-13-0] and decanal [112-31-2], and these values were higher in oils with the higher total aldehydes with 1 exception. Most values for individual aldehydes were within or below aldehyde values reported earlier.  
 IT 4674-50-4  
 RL: ANT (Analyte); ANST (Analytical study)  
 (determination of, in citrus fruit oils, gas-chromatog.)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1969:516471 HCAPLUS  
 DOCUMENT NUMBER: 71:116471  
 TITLE: Vetiveria nigritana from Angola. II. Alcohols and ketones of the essential oil  
 AUTHOR(S): Cardoso do Vale, Jose; Proenca da Cunha, Antonio  
 CORPORATE SOURCE: Port.  
 SOURCE: Garcia de Orta (1967), 15(2), 205-24  
 CODEN: GOJVA2; ISSN: 0016-4569  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Portuguese  
 AB Alcs. and ketones were studied by column chromatog. of the essential oil from the roots of V. nigritana from Angola on activated silica gel. The fraction separated by 1% MeOH in C6H6 contained a secondary alc., C15H24O, as well as ketones identified by means of anal. detns.; 2 ketones giving semicarbazones, m. 225 and 75°, were separated. The fraction obtained by elution of the column with EtOAc was mainly rich in tertiary alcs. When left undisturbed at room temperature this eluate yielded a crystalline product which on recrystn. from light petroleum ether gave a product (I), m. 154-5°, and another (II), m. 216-17°, resp. II was less abundant than I and was studied by means of thin-layer chromatog. and gas chromatog. techniques, ir spectra, and mol. weight determination

The results indicate that I is a dialc., C<sub>15</sub>H<sub>26</sub>O<sub>2</sub>, with a secondary and tertiary alc. function. The ring system of the tertiary alcs. was also elucidated through the identification of the vetivazulene obtained by dehydration of alcs. followed by dehydrogenation of the resulting hydrocarbons.

L24 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1967:414779 HCAPLUS

DOCUMENT NUMBER: 67:14779

TITLE: Terpenoids. CXV. Chemical constituents of Nardostachys jatamansi

AUTHOR(S): Sastry, S. D.; Maheshwari, M. L.; Chakravarti, Kamala K.; Bhattacharyya, Sasanka C.

CORPORATE SOURCE: Natl. Chem. Lab., Poona, India

SOURCE: Perfumery and Essential Oil Record (1967), 58(3), 154-8

CODEN: PEORAA; ISSN: 0369-8998

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 67: 3155y. The powdered roots were extracted with petroleum ether (40-60°) to yield a concrete ([α]<sub>28D</sub> +0.5°, n<sub>26D</sub> 1.4990, acid number 21.16, ester number 103.7), which was dissolved in alc., cooled to 0° for 48 hrs. to sep. the wax, and evaporated under reduced pressure to yield a solid extract which gave an acidic fraction consisting essentially of isovaleric acid; the neutral fraction (97.8%) was chromatographed on Grade III neutral alumina and eluted with petroleum ether, C<sub>6</sub>H<sub>6</sub>, Et<sub>2</sub>O, and EtOH. n-Hexacosanyl arachidate was separated from the petroleum ether fraction, and the filtrate was shown by thin-layer and gas chromatog. to contain calarene, n-hexacosane, and n-hexacosanyl isovalerate. The benzene fraction chromatographed on alumina and eluted with petroleum ether yielded valeranone, valeranal, nardol, n-hexacosanol, calarenol, nardostachone and β-sitosterol. The Et<sub>2</sub>O fraction yielded an unidentified volatile portion and a nonvolatile portion (β-sitosterol). New sesquiterpenoids identified were nardol (I), C<sub>15</sub>H<sub>26</sub>O, b<sub>0.1</sub> 120-5°, n<sub>26D</sub> 1.5005, [α]<sub>27D</sub> -10.17°; calarenol (II), C<sub>15</sub>H<sub>24</sub>O, b<sub>0.1</sub> 120-5°, [α]<sub>20D</sub> +47.9°, n<sub>26D</sub> 1.1543; and nardostachone (III), semicarbazone m. 230-2°, b<sub>0.09</sub> 130-5°, n<sub>26D</sub> 1.5571, [α]<sub>27D</sub> +209.3. The ir spectra of the sesquiterpenoids are given.

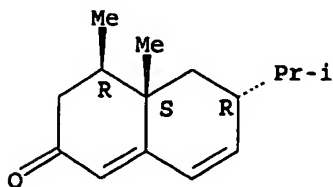
IT 15401-59-9

RL: BIOL (Biological study)  
(in Nardostachys jatamansi rhizomes)

RN 15401-59-9 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4a-dimethyl-6-(1-methylethyl)-, [4R-(4α,4α,6β)]- (9CI) (CA INDEX NAME)

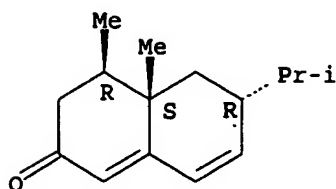
Absolute stereochemistry.



L24 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2006 ACS on STN

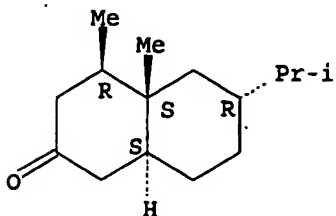
ACCESSION NUMBER: 1967:403154 HCAPLUS  
 DOCUMENT NUMBER: 67:3154  
 TITLE: Terpenoids. CVII. The structure of nardostachone  
 AUTHOR(S): Sastry, S. D.; Maheshwari, M. L.; Chakravarti, Kamala K.; Bhattacharyya, Sasanka C.  
 CORPORATE SOURCE: Natl. Chem. Lab., Poona, India  
 SOURCE: Tetrahedron (1967), 23(5), 2491-3  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI For diagram(s), see printed CA Issue.  
 AB cf. preceding abstract A new diethenoid, bicyclic ketone, C<sub>15</sub>H<sub>22</sub>O, named nardostachone, was isolated from the roots of Nardostachys jatamansi. On the basis of spectral evidences and its conversion to tetrahydronootkatone on hydrogenation, it is represented by the stereoformula I.  
 IT 15401-59-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (as structure for nardostachone)  
 RN 15401-59-9 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6-tetrahydro-4,4a-dimethyl-6-(1-methylethyl)-, [4R-(4 $\alpha$ ,4a $\alpha$ ,6 $\beta$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 20489-54-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 20489-54-7 HCAPLUS  
 CN 2(1H)-Naphthalenone, octahydro-4,4a-dimethyl-6-(1-methylethyl)-, (4R,4aS,6R,8aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> => d stat que 129 1-7  
 '1-7' IS NOT VALID HERE

=> d stat que 129

L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?

Pryor 10\_769830 Claim 76

L25           SEL PLU=ON L1 1- CHEM :       100 TERMS  
L27       133 SEA L25  
L28       133 SEA L27 OR NOOTAK?  
L29       7 SEA L28 AND (MATERIAL OR SOIL OR POLYMER? OR DIATOMACEO? OR  
          DIATOMITE OR SAND OR CELLULOSE)

=> =>

? t s3/3/1-2

3/3/1 (Item 1 from file: 5)  
DIALOG(R)File 5:Biosis Previews(R)  
(c) 2006 BIOSIS. All rts. reserv.

0014165354 BIOSIS NO.: 200300122464

Comparative effects of vetiver oil, nootkatone and disodium  
octaborate tetrahydrate on *Coptotermes formosanus* and its symbiotic  
fauna.

AUTHOR: Maistrello Lara; Henderson Gregg (Reprint); Laine Roger A  
AUTHOR ADDRESS: Agricultural Center, Department of Entomology, Louisiana  
State University, 402 Life Sciences Bldg, Baton Rouge, LA, 70803, USA\*\*  
USA

AUTHOR E-MAIL ADDRESS: GRHenderson@agctr.lsu.edu

JOURNAL: Pest Management Science 59 (1): p58-68 January 2003 2003

MEDIUM: print

ISSN: 1526-498X (ISSN print)

DOCUMENT TYPE: Article

RECORD TYPE: Abstract

LANGUAGE: English

3/3/2 (Item 2 from file: 5)  
DIALOG(R)File 5:Biosis Previews(R)  
(c) 2006 BIOSIS. All rts. reserv.

0013286669 BIOSIS NO.: 200100458508

Effects of nootkatone and a borate compound on formosan  
subterranean termite (*Isoptera: Rhinotermitidae*) and its symbiont  
protozoa

AUTHOR: Maistrello Lara (Reprint); Henderson Gregg (Reprint); Laine Roger A  
AUTHOR ADDRESS: Department of Entomology, Louisiana State University  
Agricultural Center, 402 Life Sciences Bldg., Baton Rouge, LA, 70803, USA  
\*\*USA

JOURNAL: Journal of Entomological Science 36 (3): p229-236 July, 2001 2001

MEDIUM: print

ISSN: 0749-8004

DOCUMENT TYPE: Article

RECORD TYPE: Abstract

LANGUAGE: English

?

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,  
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1296752 A1 20030402 EP 2001-945526 20010704  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2004501757 T2 20040122 JP 2002-506833 20010704  
 US 2003185956 A1 20031002 US 2003-312438 20030529  
 PRIORITY APPLN. INFO.: GB 2000-16312 A 20000704  
 WO 2001-GB3003 W 20010704

AB A method for extracting one or more desired components from a mixture in an aqueous

phase comprises separating the aqueous mixture from a water-immiscible hydrophobic

phase by means of a hydrophilic membrane and allowing the desired components to move out of the aqueous phase through the membrane and into the hydrophobic phase. The remaining components have a lower water solubility than the desired component(s), such that the remaining components are incapable of passing through the membrane. The method may be used for the isolation of materials from reaction mixts., for purification purposes or for the preparation of exts. of natural substances (flavors and aromas). Thus, selective extraction of nootkatone from grapefruit peel is attained by using a cellulose acetate dialysis membrane. Ext. may be produced in the form of carrier-based flavors, for instance absorbed on paper or maltodextrins, or encapsulated into maltodextrins, including into glass forms; which can then be formed into powders or tablets and used as such.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:678276 HCAPLUS

DOCUMENT NUMBER: 135:299936

TITLE: Effects of nootkatone and a borate compound on formosan subterranean termite (Isoptera: Rhinotermitidae) and its symbiont protozoa

AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.  
 CORPORATE SOURCE: Department of Entomology, Louisiana State University  
 Agricultural Center, Baton Rouge, LA, 70803, USA

SOURCE: Journal of Entomological Science (2001), 36(3), 229-236

CODEN: JESCEP; ISSN: 0749-8004

PUBLISHER: Georgia Entomological Society, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Wood treated with disodium octaborate tetrahydrate, with nootkatone, a natural extract isolated from vetiver oil, or with both nootkatone and disodium octaborate tetrahydrate was tested for effects on *Coptotermes formosanus* Shiraki and its hindgut flagellates. After 7 d disodium octaborate tetrahydrate-treated wood induced high termite mortality and almost complete loss of flagellates, confirming the toxicity of borates to these termites. Wood treated with nootkatone alone or with the nootkatone-borate mix was consumed in significantly lower amts. than the control, and termite survival was comparable to results obtained for starved termites. A significant progressive reduction in the total number of protozoa was observed for all groups, including the controls. Thus, nootkatone acts as a

feeding deterrent, inducing starvation that results in almost a complete loss of *Pseudotrichonympha grassii*, the most important flagellate species for cellulose digestion in this termite.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:290022 HCAPLUS  
DOCUMENT NUMBER: 134:312041  
TITLE: Apparatus for chemically compacting styrene polymer foams  
INVENTOR(S): Sakai, Tokue  
PATENT ASSIGNEE(S): Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001114927	A2	20010424	JP 1999-299017	19991021
PRIORITY APPLN. INFO.:			JP 1999-299017	19991021

AB The apparatus, useful for recycling styrene polymer foam wastes, comprises a main container part for dissolving the foam wastes in solvents (nootkatone, limonene, etc.), a lid having a device for pushing the foam wastes in the solvents, and a ring seal having a groove to fit the edge of the lid or the container, wherein the lid or the container has a groove on the edge to place the seal. Solvent leaking when the seal is swollen by the solvents is prevented with this apparatus. An illustration of the apparatus is given.

L11 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:178386 HCAPLUS  
DOCUMENT NUMBER: 134:221521  
TITLE: Process for the preparation of nootkatone by laccase catalysis  
INVENTOR(S): Huang, Rongmin; Christenson, Philip A.; Labuda, Ivica M.  
PATENT ASSIGNEE(S): Givaudan S.A., Switz.  
SOURCE: U.S., 14 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6200786	B1	20010313	US 1999-391785	19990908
ZA 2000004379	A	20010228	ZA 2000-4379	20000824
EP 1083233	A1	20010314	EP 2000-117432	20000828
EP 1083233	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 247715	E	20030915	AT 2000-117432	20000828
AU 739171	B2	20011004	AU 2000-53700	20000829
SG 87164	A1	20020319	SG 2000-4972	20000831
BR 2000004038	A	20010522	BR 2000-4038	20000906

=> d stat que

L1 33 SEA FILE=REGISTRY ABB=ON PLU=ON NOOTKATON?  
L2 SEL PLU=ON L1 1- CHEM : 100 TERMS  
L3 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L2  
L4 492 SEA FILE=HCAPLUS ABB=ON PLU=ON L3 OR NOOTKATON?  
L5 7087 SEA FILE=HCAPLUS ABB=ON PLU=ON (TICKS/CV OR ACARI/CV) OR  
TICK OR ACARI OR ANTITICK? OR ANTIACARI?  
L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND L5  
L7 194193 SEA FILE=HCAPLUS ABB=ON PLU=ON PESTICIDES/CV OR ACARICIDES/CV  
OR INSECTICIDES/CV OR RODENTICIDES/CV REPELLENTS/CV OR  
PESTICIDE OR INSECTICIDE OR RODENTICIDE OR REPELLENT  
L8 16 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND L7) NOT L6  
L9 4916981 SEA FILE=HCAPLUS ABB=ON PLU=ON MATERIAL OR SOIL OR POLYMER?  
OR DIATOMACEO? OR DIATOMITE OR SAND OR CELLULOSE  
L10 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L4(L) L9  
L11 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT (L6 OR L8)  
L15 42 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4(L) (TREAT? OR APPLY OR  
APPLIED)) NOT (L6 OR L8)  
L16 37 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L11  
L23 26 SEA FILE=HCAPLUS ABB=ON PLU=ON (L4 AND (MULCH OR GRASS OR  
ROOT OR ALUMIN? OR SILICA OR CLAY OR SOLID(W) SUBSTANC?)) NOT  
(L6 OR L8 OR L11 OR L16)  
L24 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND PD=<AUGUST 17, 2001  
L30 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND (WOOD OR CLOTH? OR  
PAPER OR COTTON? OR RUG OR CARPET? OR FLOORING OR LUMBER OR  
TEXTILE?)  
L31 20 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 NOT (L6 OR L8 OR L16 OR  
L24)  
L32 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L31 AND PD=<AUGUST 17, 2001

=> d ibib abs hitstr l32

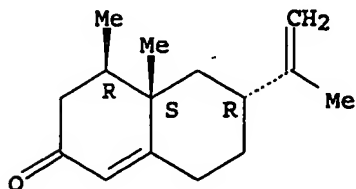
L32 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2001:678276 HCAPLUS  
DOCUMENT NUMBER: 135:299936  
TITLE: Effects of nootkatone and a borate compound  
on formosan subterranean termite (Isoptera:  
Rhinotermitidae) and its symbiont protozoa  
AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.  
CORPORATE SOURCE: Department of Entomology, Louisiana State University  
Agricultural Center, Baton Rouge, LA, 70803, USA  
SOURCE: Journal of Entomological Science (2001),  
36(3), 229-236  
CODEN: JESCEP; ISSN: 0749-8004  
PUBLISHER: Georgia Entomological Society, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Wood treated with disodium octaborate tetrahydrate, with  
nootkatone, a natural ext. isolated from vetiver oil, or with both  
nootkatone and disodium octaborate tetrahydrate was tested for  
effects on *Coptotermes formosanus* Shiraki and its hindgut flagellates.  
After 7 d disodium octaborate tetrahydrate-treated wood induced  
high termite mortality and almost complete loss of flagellates, confirming  
the toxicity of borates to these termites. Wood treated with  
nootkatone alone or with the nootkatone-borate mix was  
consumed in significantly lower amts. than the control, and termite  
survival was comparable to results obtained for starved termites. A  
significant progressive redn. in the total no. of protozoa was obsd. for  
all groups, including the controls. Thus, nootkatone acts as a  
feeding deterrent, inducing starvation that results in almost a complete  
loss of *Pseudotrichonympha grassii*, the most important flagellate species  
for cellulose digestion in this termite.  
IT 4674-50-4, Nootkatone  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)  
(effects of **nootkatone** and octaborate on formosan  
subterranean termite and its symbiont protozoa)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2-  
YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):end

=> d ibib abs hitstr 2-9

L32 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:732208 HCAPLUS

DOCUMENT NUMBER: 123:142269

TITLE: Effect of ethylene on naringin, narirutin and  
**nootkatone** accumulation in grapefruit

AUTHOR(S): Garcia Puig, D.; Perez, M. L.; Fuster, M. D.; Ortuno,  
A.; Sabater, F.; Porras, I.; Garcia Lidon, A.; Del  
Rio, J. A.

CORPORATE SOURCE: Facultad de Biologia, Univ. de Murcia, Murcia,  
E-30100, Spain

SOURCE: Planta Medica (1995), 61(3), 283-5

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper studies the effect of different concns. of ethephon  
on the levels of the sesquiterpene, **nootkatone**, and of the  
flavanones, naringin and narirutin, in grapefruit. **Nootkatone**  
synthesis and/or accumulation was stimulated by all the concns. of  
ethephon assayed, while the levels of naringin and narirutin in the rind  
diminished. These results open up new perspectives concerning the  
possible regulation of the secondary metab. of the plants.

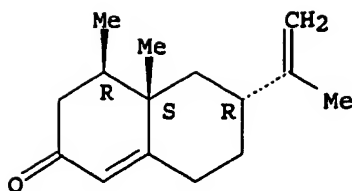
IT 4674-50-4, **Nootkatone**

RL: BPR (Biological process); BSU (Biological study, unclassified); MFM  
(Metabolic formation); BIOL (Biological study); FORM (Formation,  
nonpreparative); PROC (Process)  
(effect of ethylene on naringin, narirutin and **nootkatone**  
accumulation in grapefruit)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:730353 HCAPLUS

DOCUMENT NUMBER: 123:138818

TITLE: Identification of wood species in conifer wood

AUTHOR(S): Hiraki, Toshikazu; Kota, Masahito; Kawaguch, Toshimune; Ikehara, Yukari; Arime, Masaaki; Satou, Souei

CORPORATE SOURCE: Osaka Customs Laboratory, Osaka, 552, Japan

SOURCE: Kanzei Chuo Bunsekishoho (1995), 34, 105-20

CODEN: KCBSDI; ISSN: 0286-1933

PUBLISHER: Okurasho Kanzei Chuo Bunsekisho

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB For the identification of the species in conifer wood, their exts. from woods with n-hexane were analyzed by gas-chromatog. and mass-spectrometry method (GC-MS method). In addn., the observation of wood tissue by microscopy was also examd. The total ion chromatogram patterns of their exts. exhibited characteristic pattern depending on the species of these woods. Specific components detected in some wood species were used for identification of conifer woods; todomatuic acid Me ester from Todo-Matsu, nootkatone from Yellow Cedar and nezukone from Western Red Cedar. Characteristic structures of wood tissue were obsd. by microscopy for the discrimination of these wood species. Thus, GC-MS and microscopic methods were very useful for the indentification of the species in conifer wood.

IT 4674-50-4, Nootkatone

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

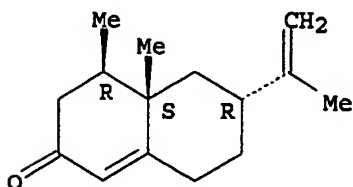
BIOL (Biological study); OCCU (Occurrence)

(identification of constituents of conifer species)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:319389 HCAPLUS

DOCUMENT NUMBER: 120:319389

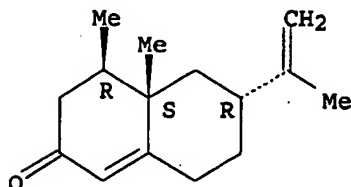
TITLE: Extraction of volatile compounds from conifer woods with supercritical carbon dioxide

AUTHOR(S): Terauchi, Fumio; Ohira, Tatsuro; Yatagai, Mitsuyoshi; Ohgama, Toshimasa; Aoki, Hiroyuki; Suzuki, Tsutomu

CORPORATE SOURCE: Grad. Sch. Sci. Technol., Chiba Univ., Chiba, 263,

SOURCE: Japan  
 Mokuzaigakkaishi (1993), 39(12), 1421-30  
 CODEN: MKZGA7; ISSN: 0021-4795  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Japanese  
 AB Supercrit. fluid extn. (SFE) with carbon dioxide and hot-water distn. were conducted using the woods of *Chamaecyparis obtusa* Endl. (hinoki), *Thujopsis dolabrata* var. *handai* Makino (hinokiasunaro), *Chamaecyparis nootkatensis* Spach (Alaska cedar), *Thuja plicata* D. Don. (western red cedar), *Pinus densiflora* S. et Z. (akamatsu), *Pseudotsuga menziesii* Franco (Douglas-fir), and *Cryptomeria japonica* D. Don (sugi). The yields by SFE (30 min) were more than those obtained by hot-water distn. for 8 h, except for Alaska cedar. The yields at 300 kgf/cm<sup>2</sup> were about twice as high as those at 100 kgf/cm<sup>2</sup>, and as extn. time increased, the yield increased. The components of SFE exts. and essential oils by hot-water distns. were identified by gas liq. chromatog. and gas chromatog.-mass spectrometry. The compn. of the SFE exts. from hinoki, sugi, akamatsu, and hinokiasunaro were qual. similar to those of essential oils obtained by hot-water distn. Although the contents of high-mol.-wt. compds. and terpene hydrocarbons were a little greater in SFE exts. than in essential oils obtained by hot-water distn. Western red cedar and Douglas-fir woods were extd. selectively by SFE, and the compns. of SFE exts. were quite different from the essential oils obtained by hot-water distn.  
 IT 4674-50-4, Nootkatone  
 RL: PROC (Process)  
 (extn. of, from conifer woods with supercrit. carbon dioxide)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

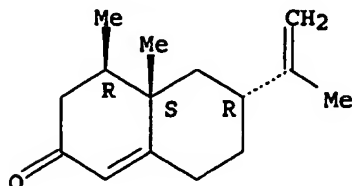
Absolute stereochemistry.



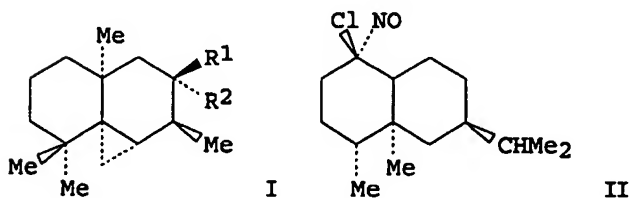
L32 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1994:173092 HCAPLUS  
 DOCUMENT NUMBER: 120:173092  
 TITLE: Minor components in the essential oil of *Juniperus oxycedrus* L. wood  
 AUTHOR(S): Barrero, Alejandro F.; Oltra, J. Enrique; Altarejos, Joaquin; Barragan, Armando; Lara, Armando; Laurent, Raymond  
 CORPORATE SOURCE: Fac. Cienc., Univ. Granada, Granada, 18071, Spain  
 SOURCE: Flavour and Fragrance Journal (1993), 8(4), 185-9  
 CODEN: FFJOED; ISSN: 0882-5734  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A detailed study of the essential oil from the wood of *Juniperus oxycedrus* L. allowed the identification of 42 components, 15 of them being reported the first time in this oil.  
 IT 4674-50-4, Nootkatone  
 RL: BIOL (Biological study)  
 (of *Juniperus oxycedrus* wood oil)  
 RN 4674-50-4 HCAPLUS  
 CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-

methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1992:571728 HCAPLUS  
DOCUMENT NUMBER: 117:171728  
TITLE: Sesquiterpenes. Carbon-13 and proton NMR chemical shifts of new thujopsane and nootkatane derivatives.  
AUTHOR(S): Wolff, Peter  
CORPORATE SOURCE: Ruhr-Univ. Bochum, Bochum, 4630/1, Germany  
SOURCE: Magnetic Resonance in Chemistry (1992), 30(8), 803-4  
CODEN: MRCHEG; ISSN: 0749-1581  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

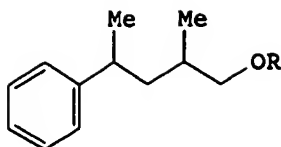


AB The <sup>13</sup>C- and <sup>1</sup>H-NMR spectra of thujopsanone oxime (I; R1R2 = NOH), 7-halo-7-nitrosothujopsanes (I; R1 = Cl, Br, R2 = NOH), nootkat-1-one oxime and 1-chloro-1-nitrosoneootkatane (II) are reported.

L32 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1987:72732 HCAPLUS  
DOCUMENT NUMBER: 106:72732  
TITLE: Uses of 2-methyl-4-phenyl-1-pentanol derivatives in augmenting or enhancing the aroma or taste of consumable materials  
INVENTOR(S): Hall, John B.  
PATENT ASSIGNEE(S): International Flavors and Fragrances Inc., USA  
SOURCE: U.S., 26 pp. Division of U.S. Ser. No. 681,656.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4610812	A	19860909	US 1985-784059	19851004 <--
US 4650898	A	19870317	US 1984-681656	19841214 <--
PRIORITY APPLN. INFO.:			US 1984-681656	A3 19841214

GI



AB Pentanol derivs. I (R = H, Ac) are added to consumable materials, e.g. perfume compns., colognes, perfumed articles, foodstuffs, chewing gums, medicinal products, and chewing tobacco, to augment or enhance the aroma or taste. I (R = H) has a powerful long-lasting stable green grapefruit-like, nootkatone-like, animalic, leathery, vetiver-like, olibanum, musky and floral aroma profile; and a floral, green, weedy, fruity, grapefruit, galbanum-like aroma and taste at 1 ppm. I (R = Ac) has a green, styrallyl acetate-like aroma; and a floral, nootkatone-like, oriental, green pepper-like aroma and taste at 1 ppm. I (R = H) was prepd. by condensation of propanal with hydratropic aldehyde to give a mixt. contg. isomeric 2-methyl-4-pentenals, which were hydrogenated using Raney Ni catalyst. I (R = H) was acetylated with Ac2O in presence of conc. H3PO4 to give I (R = Ac). A herbal perfume formulation contained Oakmoss abs. 20, 2-methyl-3,4-(methylenedioxy)hydrocinnamic aldehyde 10, Me dihydrojasmonate 100 coumarin 20, musk ketone 80, isocyclocitral 10, galbanum oil 6 rosemary oil 10, pine needle oil 60, fir balsam abs. 10, bergamot oil 60, lemon oil 14, benzyl acetate 468, linalool 80, indole 6, undecalactone 12 and I (R = H) 12 parts by wt.

L32 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:89951 HCAPLUS  
DOCUMENT NUMBER: 76:89951  
TITLE: Odor and molecular structure  
AUTHOR(S): Teranishi, R.  
CORPORATE SOURCE: West. Util. Res. Dev. Div., Agric. Res. Serv., Albany, CA, USA  
SOURCE: Gustation Olfaction, Int. Symp. (1971), Meeting Date 1970, 165-77. Editor(s): Ohloff, Guenther. Academic: London, Engl.  
CODEN: 24IDA7  
DOCUMENT TYPE: Conference  
LANGUAGE: English

AB Small changes in the chem. structure of musk-, amber-, and wood -type odor compds. change the potency greatly but not the quality. In the case of nootkatone and related compds. the quality changes but the potency remains relatively unchanged. 2-Methoxy-3-isobutylpyrazine, the characteristic, highly potent odor component of green bell peppers, has an unusually high odor potency even among the enantiomers.

L32 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:509933 HCAPLUS  
DOCUMENT NUMBER: 73:109933  
TITLE: Nootkatone from nootkatene  
INVENTOR(S): Ohloff, Guenther  
PATENT ASSIGNEE(S): Firmenich et Cie.  
SOURCE: Ger. Offen., 13 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1948033	A	19700903	DE 1969-1948033	19690923 <--
CH 502291	A	19710131	CH 1968-502291	19680925 <--
FR 2018838	AS	19700626	FR 1969-32534	19690924 <--
NL 6914545	A	19700331	NL 1969-14545	19690925 <--
GB 1208090	A	19701007	GB 1969-1208090	19690925 <--
SE 356968	B	19730612	SE 1969-13198	19690925 <--
PRIORITY APPLN. INFO.:			CH 1968-14342	A 19680925

GI For diagram(s), see printed CA Issue.

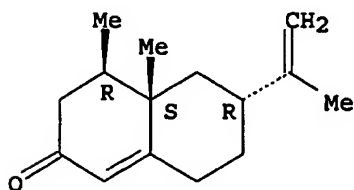
AB Nootkatone (I) was prepd. from nootkatone (II) by hydrochlorination and subsequent oxidn. with Na<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> or Jones' reagent. I was useful as grapefruit-like flavor. Thus, II was isolated from the wood of *Chamaecyparis nootkatensis* by steam distn. and chromatog. of the org. layer. A II soln. in Et<sub>2</sub>O was satd. with gaseous HCl at -10 to 0.degree.. Jones' reagent was added to give after 60 hr 80% I.

IT 4674-50-4P  
RL: PREP (Preparation)  
(from nootkatene)

RN 4674-50-4 HCAPLUS

CN 2(3H)-Naphthalenone, 4,4a,5,6,7,8-hexahydro-4,4a-dimethyl-6-(1-methylethenyl)-, (4R,4aS,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



? t s3/3/1-2

3/3/1 (Item 1 from file: 5)  
DIALOG(R)File 5:Biosis Previews(R)  
(c) 2006 BIOSIS. All rts. reserv.

0014165354 BIOSIS NO.: 200300122464  
Comparative effects of vetiver oil, nootkatone and disodium  
octaborate tetrahydrate on Coptotermes formosanus and its symbiotic  
fauna.  
AUTHOR: Maistrello Lara; Henderson Gregg (Reprint); Laine Roger A  
AUTHOR ADDRESS: Agricultural Center, Department of Entomology, Louisiana  
State University, 402 Life Sciences Bldg, Baton Rouge, LA, 70803, USA\*\*  
USA  
AUTHOR E-MAIL ADDRESS: GRHenderson@agctr.lsu.edu  
JOURNAL: Pest Management Science 59 (1): p58-68 January 2003 2003  
MEDIUM: print  
ISSN: 1526-498X (ISSN print)  
DOCUMENT TYPE: Article  
RECORD TYPE: Abstract  
LANGUAGE: English

3/3/2 (Item 2 from file: 5)  
DIALOG(R)File 5:Biosis Previews(R)  
(c) 2006 BIOSIS. All rts. reserv.

0013286669 BIOSIS NO.: 200100458508  
Effects of nootkatone and a borate compound on formosan  
subterranean termite (Isoptera: Rhinotermitidae) and its symbiont  
protozoa  
AUTHOR: Maistrello Lara (Reprint); Henderson Gregg (Reprint); Laine Roger A  
AUTHOR ADDRESS: Department of Entomology, Louisiana State University  
Agricultural Center, 402 Life Sciences Bldg., Baton Rouge, LA, 70803, USA  
\*\*USA  
JOURNAL: Journal of Entomological Science 36 (3): p229-236 July, 2001 2001  
MEDIUM: print  
ISSN: 0749-8004  
DOCUMENT TYPE: Article  
RECORD TYPE: Abstract  
LANGUAGE: English  
?

RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,  
 UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1296752 A1 20030402 EP 2001-945526 20010704

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2004501757 T2 20040122 JP 2002-506833 20010704

US 2003185956 A1 20031002 US 2003-312438 20030529

PRIORITY APPLN. INFO.:

GB 2000-16312 A 20000704

WO 2001-GB3003 W 20010704

AB A method for extracting one or more desired components from a mixture in an aqueous

phase comprises separating the aqueous mixture from a water-immiscible hydrophobic

phase by means of a hydrophilic membrane and allowing the desired components to move out of the aqueous phase through the membrane and into the hydrophobic phase. The remaining components have a lower water solubility than the desired component(s), such that the remaining components are incapable of passing through the membrane. The method may be used for the isolation of materials from reaction mixts., for purification purposes or for the preparation of exts. of natural substances (flavors and aromas). Thus, selective extraction of nootkatone from grapefruit peel is attained by using a cellulose acetate dialysis membrane. Ext. may be produced in the form of carrier-based flavors, for instance absorbed on paper or maltodextrins, or encapsulated into maltodextrins, including into glass forms; which can then be formed into powders or tablets and used as such.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:678276 HCAPLUS

DOCUMENT NUMBER: 135:299936

TITLE: Effects of nootkatone and a borate compound on formosan subterranean termite (Isoptera:

Rhinotermitidae) and its symbiont protozoa

AUTHOR(S): Maistrello, Lara; Henderson, Gregg; Laine, Roger A.  
 CORPORATE SOURCE: Department of Entomology, Louisiana State University  
 Agricultural Center, Baton Rouge, LA, 70803, USA

SOURCE: Journal of Entomological Science (2001), 36(3),  
 229-236

CODEN: JESCEP; ISSN: 0749-8004

PUBLISHER: Georgia Entomological Society, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Wood treated with disodium octaborate tetrahydrate, with nootkatone, a natural extract isolated from vetiver oil, or with both nootkatone and disodium octaborate tetrahydrate was tested for effects on Coptotermes formosanus Shiraki and its hindgut flagellates. After 7 d disodium octaborate tetrahydrate-treated wood induced high termite mortality and almost complete loss of flagellates, confirming the toxicity of borates to these termites. Wood treated with nootkatone alone or with the nootkatone-borate mix was consumed in significantly lower amts. than the control, and termite survival was comparable to results obtained for starved termites. A significant progressive reduction in the total number of protozoa was observed for all groups, including the controls. Thus, nootkatone acts as a

feeding deterrent, inducing starvation that results in almost a complete loss of *Pseudotrichonympha grassii*, the most important flagellate species for cellulose digestion in this termite.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:290022 HCAPLUS

DOCUMENT NUMBER: 134:312041

TITLE: Apparatus for chemically compacting styrene polymer foams

INVENTOR(S): Sakai, Tokue

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001114927	A2	20010424	JP 1999-299017	19991021
PRIORITY APPLN. INFO.:			JP 1999-299017	19991021

AB The apparatus, useful for recycling styrene polymer foam wastes, comprises a main container part for dissolving the foam wastes in solvents (nootkatone, limonene, etc.), a lid having a device for pushing the foam wastes in the solvents, and a ring seal having a groove to fit the edge of the lid or the container, wherein the lid or the container has a groove on the edge to place the seal. Solvent leaking when the seal is swollen by the solvents is prevented with this apparatus. An illustration of the apparatus is given.

L11 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:178386 HCAPLUS

DOCUMENT NUMBER: 134:221521

TITLE: Process for the preparation of nootkatone by laccase catalysis

INVENTOR(S): Huang, Rongmin; Christenson, Philip A.; Labuda, Ivica M.

PATENT ASSIGNEE(S): Givaudan S.A., Switz.

SOURCE: U.S., 14 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6200786	B1	20010313	US 1999-391785	19990908
ZA 2000004379	A	20010228	ZA 2000-4379	20000824
EP 1083233	A1	20010314	EP 2000-117432	20000828
EP 1083233	B1	20030820		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 247715	E	20030915	AT 2000-117432	20000828
AU 739171	B2	20011004	AU 2000-53700	20000829
SG 87164	A1	20020319	SG 2000-4972	20000831
BR 2000004038	A	20010522	BR 2000-4038	20000906